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Supporting Information

A straight forward synthesis of 4-aryl substituted 2-quinolone via Heck reaction

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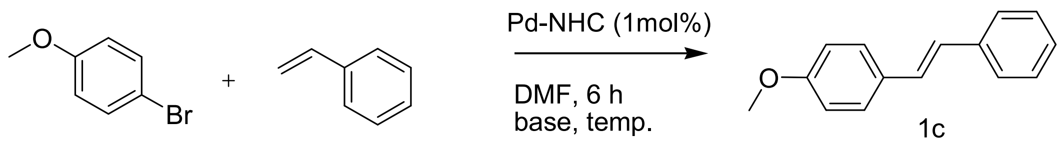
Experimental

Table- S1: Optimization for reaction between 4-bromoanisole and styrene[a]



Entry	Base	Temp. (^oC)	Yield (%)[b]
1	Et_3N	90	35
2	Et_3N	110	42
3	Et_3N	130	65
4	K_2CO_3	130	86
5	Cs_2CO_3	130	N.R.
6	NaOAc	130	<20

[a]Reaction conditions: 4-bromoanisole (1 mmol), styrene (1.5 mmol), base (2 mmol), Pd-NHC (1 mol%, 0.0096g), DMF, 6 hr; [b]Isolated yield after column chromatography.

Spectral analysis:

n-Butyl-3-(4-methoxyphenyl)acrylate (1a)[1]

Yellowish liquid; ^1H NMR ($CDCl_3$, 300 MHz) δ : 0.96 (t, J = 7.2 Hz, 3H), 1.37-1.50 (m, 2H), 1.64-1.73 (m, 2H), 3.88 (s, 3H), 4.20 (t, J = 6.9 Hz, 2H), 6.31 (d, J = 16.2 Hz, 1H), 6.90 (d, J = 8.7 Hz, 2H), 7.48 (d, J = 9 Hz, 2H), 7.64 (d, J = 15.9 Hz, 1H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ : 13.78, 19.22, 30.80, 55.37, 64.28, 114.28, 115.73, 127.18, 129.70, 144.23, 161.30, 167.49.

3-(4-methoxyphenyl)acrylonitrile (1b)[2]

Yellowish liquid; ^1H NMR ($CDCl_3$, 300 MHz) δ : 3.84 (s, 3H), 5.71 (d, J = 16.8 Hz, 1H), 6.90-6.93 (m, 2H), 7.30-7.41(m, 4H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ : 55.42, 93.32, 114.48, 118.66, 126.31, 129.04, 150.01, 162.01.

1-(4-methoxystyryl)benzene (1c)[3]

White solid; m.p. 135-137^{o}C; ^1H NMR ($CDCl_3$, 300 MHz) δ : 3.75 (s, 3H), 6.80-6.87 (m, 2H), 6.94 (d, J = 14.4 Hz, 1H), 7.13-7.18 (m, 2H), 7.21-7.29 (m, 3H), 7.35-7.42 (m, 3H); ^{13}C

NMR ($CDCl_3$, 75MHz) δ : 55.35, 114.14, 126.27, 126.62, 127.24, 127.74, 128.21, 128.67, 130.15, 137.65, 159.30.

n-Butyl-3-*p*-tolylacrylate (1d)[1]

Yellow liquid; ^{1}H NMR ($CDCl_3$, 300 MHz) δ : 0.96 (t, J = 7.2 Hz, 3H), 1.38-1.50 (m, 2H), 1.64-1.73 (m, 2H), 2.37 (s, 3H), 4.20 (t, J = 6.9 Hz, 2H), 6.39 (d, J = 15.9 Hz, 1H), 7.19 (d, J = 7.8 Hz, 2H), 7.42 (d, J = 8.1 Hz, 2H), 7.66 (d, J = 15.9 Hz, 1H); ^{13}C NMR ($CDCl_3$, 75MHz) δ : 13.77, 19.21, 21.46, 30.79, 64.35, 117.18, 128.04, 129.60, 131.73, 140.61, 144.55, 167.32.

Ethyl-3-(2-fluorophenyl)acrylate (1e)[4]

Light yellow liquid; ^{1}H NMR ($CDCl_3$, 300 MHz) δ : 1.32 (t, J = 7.2 Hz, 3H), 4.25 (q, J = 7.2 Hz, 2H), 6.52 (d, J = 16.2 Hz, 1H), 7.03-7.16 (m, 1H), 7.29-7.36 (m,1H), 7.48-7.54 (m, 1H), 7.79 (d, J = 16.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 75MHz) δ : 14.02, 60.34, 115.89 (d, $J_{C\text{-}F}$ = 21.82 Hz), 120.55 (d, $J_{C\text{-}F}$ = 6.52 Hz), 122.21 (d, $J_{C\text{-}F}$ = 11.7 Hz), 124.15 (d, $J_{C\text{-}F}$ = 3.67 Hz), 128.74 (d, $J_{C\text{-}F}$ = 2.77 Hz), 131.36 (d, $J_{C\text{-}F}$ = 8.7 Hz), 136.87 (d, $J_{C\text{-}F}$ = 2.85 Hz), 161.04 (d, $J_{C\text{-}F}$ = 252.37 Hz), 166.53.

1-(4-chlorostyryl)benzene (1f)[3]

White solid; m.p. 128-130°C; ^{1}H NMR ($CDCl_3$, 300 MHz) δ : 7.03 (d, J = 1.5 Hz, 2H), 7.20-7.49 (m, 9H); ^{13}C NMR ($CDCl_3$, 75MHz) δ : 126.61, 127.39, 127.72, 127.93, 128.79, 128.89, 129.34, 133.20, 135.87, 137.01.

3-*o*-tolylacrlonitrile (1g)[2]

Light yellow liquid; ^{1}H NMR ($CDCl_3$, 300 MHz) δ : 2.37 (s, 3H), 5.76 (d, J = 16.5 Hz, 1H), 7.17-7.32 (m, 3H), 7.39-7.44 (m, 1H), 7.66 (d, J = 16.5 Hz, 1H); ^{13}C NMR ($CDCl_3$, 75MHz) δ : 19.38, 96.95, 118.16, 125.30, 126.36, 130.75, 130.79, 132.29, 136.99, 148.21.

Methyl-3-(2-aminophenyl)acrylate (1h)[5]

Yellow solid; m.p. 59-61°C; ^{1}H NMR ($CDCl_3$, 300 MHz) δ : 3.72 (s, 3H), 3.87 (s, 2H), 6.28 (d, J = 15.9 Hz, 1H), 6.61-6.71 (m, 2H), 7.06-7.12 (m, 1H), 7.30 (dd, J = 7.8, 1.5 Hz, 1H), 7.77 (d, J = 15.9 Hz, 1H); ^{13}C NMR ($CDCl_3$, 75MHz) δ : 51.65, 116.82, 117.56, 118.93, 119.83, 128.06, 131.36, 140.37, 145.67, 167.76.

n-Butyl-3-(napthalen-1-yl)acrylate (1i)[1]

Light yellow liquid; ^{1}H NMR ($CDCl_3$, 300 MHz) δ : 0.97 (t, J = 7.2 Hz, 3H), 1.39-1.51 (m, 2H), 1.62-1.76 (m, 2H), 4.23 (t, J = 6.6 Hz, 2H), 6.51 (d, J = 15.6 Hz, 1H), 7.43-7.56 (m, 3H), 7.71 (d, J = 7.2 Hz, 1H), 7.75-7.85 (m, 2H), 8.16 (d, J = 8.1 Hz, 1H), 8.51 (d, J = 15.6

Hz, 1H); ^{13}C NMR ($CDCl_3$, 75MHz) δ : 13.84, 19.29, 30.86, 64.57, 120.93, 123.40, 125.01, 125.47, 126.23, 126.87, 128.75, 130.49, 131.43, 131.82, 133.70, 141.60, 167.03.

Ethyl-3-(2-hydroxyphenyl)acrylate (1j)[6]

Light yellow liquid; ^{1}H NMR ($CDCl_3$, 300 MHz) δ : 1.35 (t, J = 7.2 Hz, 3H), 4.30 (q, J = 7.2 Hz, 2H), 6.67 (dd, J = 16.2, 1.2 Hz, 1H), 6.87-6.92 (m, 2H), 7.19-7.25 (m, 1H), 7.45 (dd, J = 8.1, 1.5 Hz, 2H), 8.08 (d, J = 16.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 75MHz) δ : 14.31, 60.86, 116.50, 118.08, 120.52, 121.69, 129.20, 131.51, 141.15, 155.81, 168.96.

n-Butyl-3-(3-methylphenyl)acrylate (1k)[7]

Light yellow oil; ^{1}H NMR ($CDCl_3$, 300 MHz) δ : 0.98 (t, 3H), 1.39-1.49 (m, 2H), 1.63-1.72 (m, 2H), 2.34 (s, 3H), 4.20 (t, J = 6.6 Hz, 2H), 6.41 (d, J = 15.9 Hz, 1H), 7.15-7.31 (m, 4H), 7.64 (d, J = 15.9 Hz, 1H); ^{13}C NMR ($CDCl_3$, 75MHz) δ : 13.76, 19.23, 21.28, 30.81, 64.35, 118.05, 125.25, 128.71, 128.74, 131.04, 134.43, 138.47, 144.72, 167.12.

Methyl-3-(3-methoxylphenyl)acrylate (1l)[8]

Light yellow oil; ^{1}H NMR ($CDCl_3$, 300 MHz) δ : 3.80 (s, 6H), 6.42 (d, J = 15.9 Hz, 1H), 6.90-6.93 (m, 1H), 7.01-7.03 (m, 1H), 7.09 (d, J = 7.8 Hz, 1H), 7.25-7.30 (m, 1H), 7.64 (d, J = 15.9 Hz, 1H); ^{13}C NMR ($CDCl_3$, 75MHz) δ : 51.66, 55.23, 113.00, 116.10, 118.03, 120.73, 129.87, 135.72, 144.77, 159.89, 167.34.

1-(4-fluorostyryl)benzene (1m)[3]

White solid; m.p. 122-124^{o}C; ^{1}H NMR ($CDCl_3$, 300 MHz) δ : 6.97-7.09 (m, 4H), 7.22-7.28 (m, 1H), 7.33-7.38 (m, 2H), 7.44-7.50 (m, 4H); ^{13}C NMR ($CDCl_3$, 75MHz) δ : 115.67 (d, $J_{C\text{-}F}$ = 21.5 Hz), 126.49, 127.48, 127.73, 128.03 (d, $J_{C\text{-}F}$ = 7.9 Hz), 128.46, 128.77, 133.51 (d, $J_{C\text{-}F}$ = 3.3 Hz), 137.17, 162.35 (d, $J_{C\text{-}F}$ = 245.5 Hz).

1-(4-styrylphenyl)ethanone (1n)[3]

White solid; m.p. 141-143^{o}C; ^{1}H NMR ($CDCl_3$, 300 MHz) δ : 2.60 (s, 3H), 7.09-7.20 (m, 2H), 7.25-7.32 (m, 1H), 7.35-7.40 (m, 2H), 7.52-7.59 (m, 4H), 7.94 (d, J = 8.4 Hz); ^{13}C NMR ($CDCl_3$, 75MHz) δ : 26.60, 126.51, 126.83, 127.45, 128.33, 128.81, 128.89, 131.48, 135.95, 136.70, 142.03, 197.52.

4-styrylbenzonitrile (1o)[3]

White solid; m.p. 114-116^{o}C; ^{1}H NMR ($CDCl_3$, 300 MHz) δ : 7.07 (d, J = 16.5 Hz, 1H), 7.20 (d, J = 16.5 Hz, 1H), 7.31-7.41 (m, 3H), 7.52-7.63 (m, 6H); ^{13}C NMR ($CDCl_3$, 75MHz) δ : 110.62, 119.02, 126.75, 126.88, 126.94, 128.66, 128.87, 132.44, 132.48, 136.32, 141.86.

4-(4-methoxyphenyl)quinolin-2-(*1H*)-one (2a)[9]

White solid; m.p. 196-198°C; ^{1}H NMR ($CDCl_3$, 300 MHz) δ : 3.99 (s, 3H), 6.81 (s, 1H), 7.14 (d, *J* = 8.7 Hz, 2H), 7.27-7.37 (m, 1H), 7.52 (d, *J* = 8.7 Hz, 2H), 7.65 (d, *J* = 6 Hz, 2H), 7.74 (d, *J* = 8.1 Hz, 1H), 12.7 (bs, 1H); ^{13}C NMR ($CDCl_3$, 75MHz) δ : 55.41, 114.14, 116.80, 119.96, 120.08, 122.78, 126.86, 129.31, 130.24, 130.79, 138.74, 153.57, 160.26, 163.94.

4-*p*-tolylquinolin-2(*1H*)-one (2b)[9]

White solid; m.p. 229-231°C; ^{1}H NMR ($CDCl_3$, 300 MHz) δ : 2.46 (s, 3H), 6.71 (s, 1H), 7.14-7.19 (m, 1H), 7.31-7.39 (m, 4H), 7.50-7.61 (m, 3H), 13.00 (bs, 1H); ^{13}C NMR ($CDCl_3$, 75MHz) δ : 21.36, 116.85, 119.76, 120.42, 122.61, 126.79, 128.84, 129.34, 130.71, 134.21, 138.86, 138.93, 153.69, 164.36.

4-*m*-tolylquinolin-2(*1H*)-one (2c)[10]

White solid; m.p. 158-160°C; ^{1}H NMR ($CDCl_3$, 300 MHz) δ : 2.45 (s, 3H), 6.72 (s, 1H), 7.17-7.22 (m, 1H), 7.26-7.32 (m, 3H), 7.41 (t, *J* = 7.8 Hz, 1H), 7.55-7.61 (m, 3H), 12.60 (bs, 1H); ^{13}C NMR ($CDCl_3$, 75MHz) δ : 21.52, 116.81, 119.86, 120.21, 122.86, 125.98, 126.92, 128.54, 129.51, 129.66, 130.87, 136.94, 138.44, 138.65, 154.09, 163.93.

4-(3-methoxyphenyl)quinolin-2(*1H*)-one (2d)[9]

White solid; m.p. 190-192°C; ^{1}H NMR ($CDCl_3$, 300 MHz) δ : 3.87 (s, 3H), 6.74 (s, 1H), 7.02-7.07 (m, 3H), 7.18 (m, 1H), 7.43 (t, *J* = 7.8 Hz, 1H), 7.54-7.62 (m, 3H), 12.90 (bs, 1H); ^{13}C NMR ($CDCl_3$, 75MHz) δ : 55.41, 114.42, 114.45, 116.84, 119.63, 120.52, 121.28, 122.73, 126.77, 129.73, 130.81, 138.42, 138.86, 153.52, 159.66, 164.42.

4-(2-methoxyphenyl)quinolin-2(*1H*)-one (2e)

White solid; m.p. 210-212°C; ^{1}H NMR ($CDCl_3$, 300 MHz) δ: 3.64 (s, 3H), 6.61 (s, 1H), 6.94-7.04 (m, 3H), 7.15-7.19 (m, 2H), 7.34-7.47 (m, 3H), 12.90 (bs, 1H); ^{13}C NMR ($CDCl_3$, 75MHz) δ : 55.53, 111.10, 116.59, 120.12, 120.79, 121.55, 122.33, 126.08, 126.91, 130.27, 130.40, 130.55, 138.46, 151.13, 156.58, 164.57; MS (ESI+): m/z 251.80 $[M]^+$; elemental analysis calcd (%) for $C_{16}H_{13}NO_2$: C, 76.48; H, 5.21; N, 5.57, found C, 76.41; H, 5.15; N, 5.61.

4-*o*-tolylquinolin-2(*1H*)-one (2f)

White solid; m.p. 178-180°C; ^{1}H NMR ($CDCl_3$, 300 MHz) δ : 2.05 (s, 3H), 6.56 (s, 1H), 6.99-7.06 (m, 2H), 7.11-7.16 (m, 1H), 7.22-7.32 (m, 3H), 7.39-7.49 (m, 2H), 12.92 (bs, 1H); ^{13}C NMR ($CDCl_3$, 75MHz) δ: 19.85, 116.67, 120.07, 120.91, 122.73, 125.93, 126.67, 128.65, 128.93, 130.29, 130.78, 135.68, 136.64, 138.59, 153.65, 164.55; MS (ESI+): m/z 235.80

[M]$^+$; elemental analysis calcd (%) for $C_{16}H_{13}NO$: C, 81.68; H, 5.57; N, 5.95, found C, 81.57; H, 5.51; N, 5.98.

4-(4-chlorophenyl)quinolin-2(*1H*)-one (2g)[10]

White solid; m.p. 208-210°C; ^{1}H NMR (DMSO-d_6, 300 MHz) δ : 6.30 (s, 1H), 7.00-7.06 (m, 1H), 7.22-7.30 (m, 2H), 7.38-7.48 (m, 5H), 11.80 (s,1H); ^{13}C NMR (DMSO-d_6, 75 MHz) δ : 116.29, 118.57, 121.92, 122.45, 126.44, 129.21, 131.08, 131.17, 134.09, 135.94, 139.73, 150.70, 161.66.

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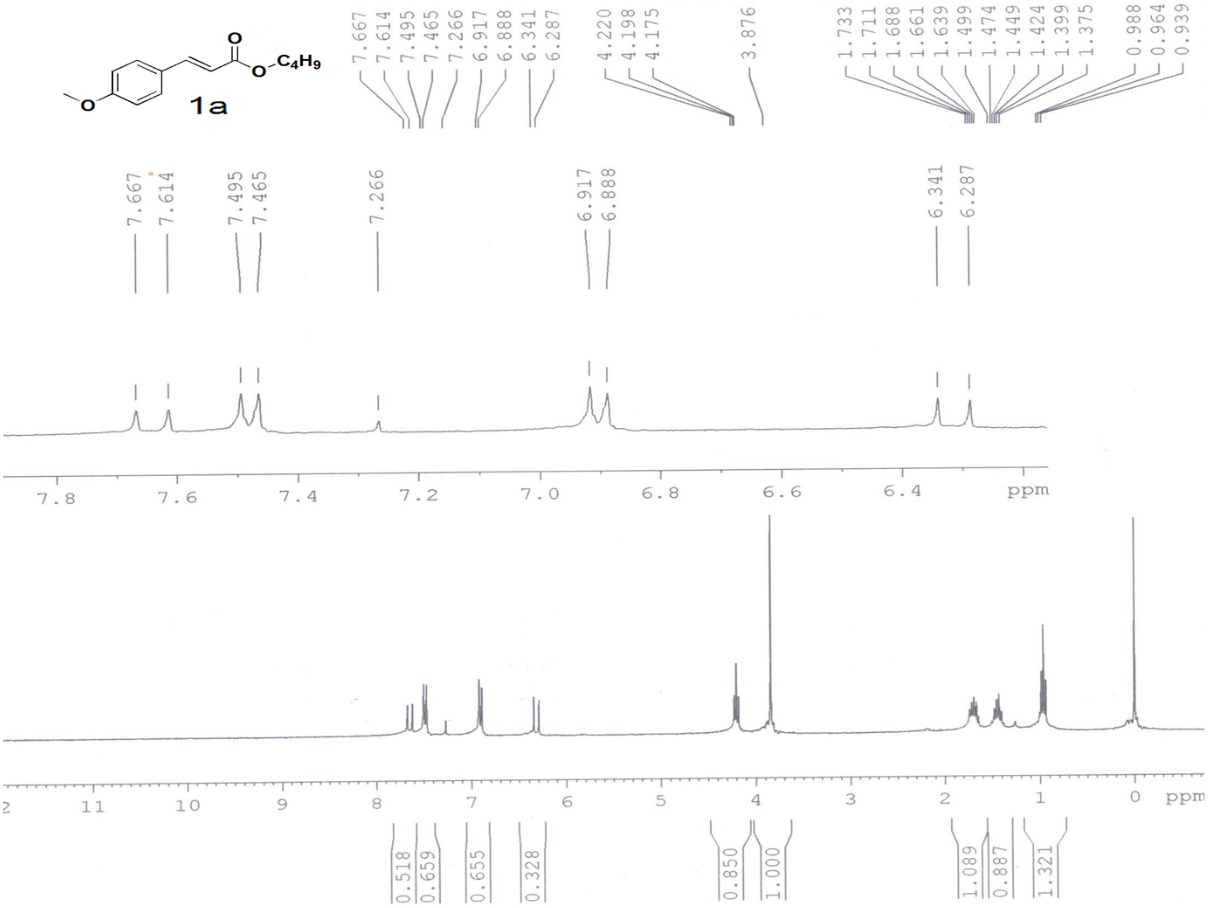
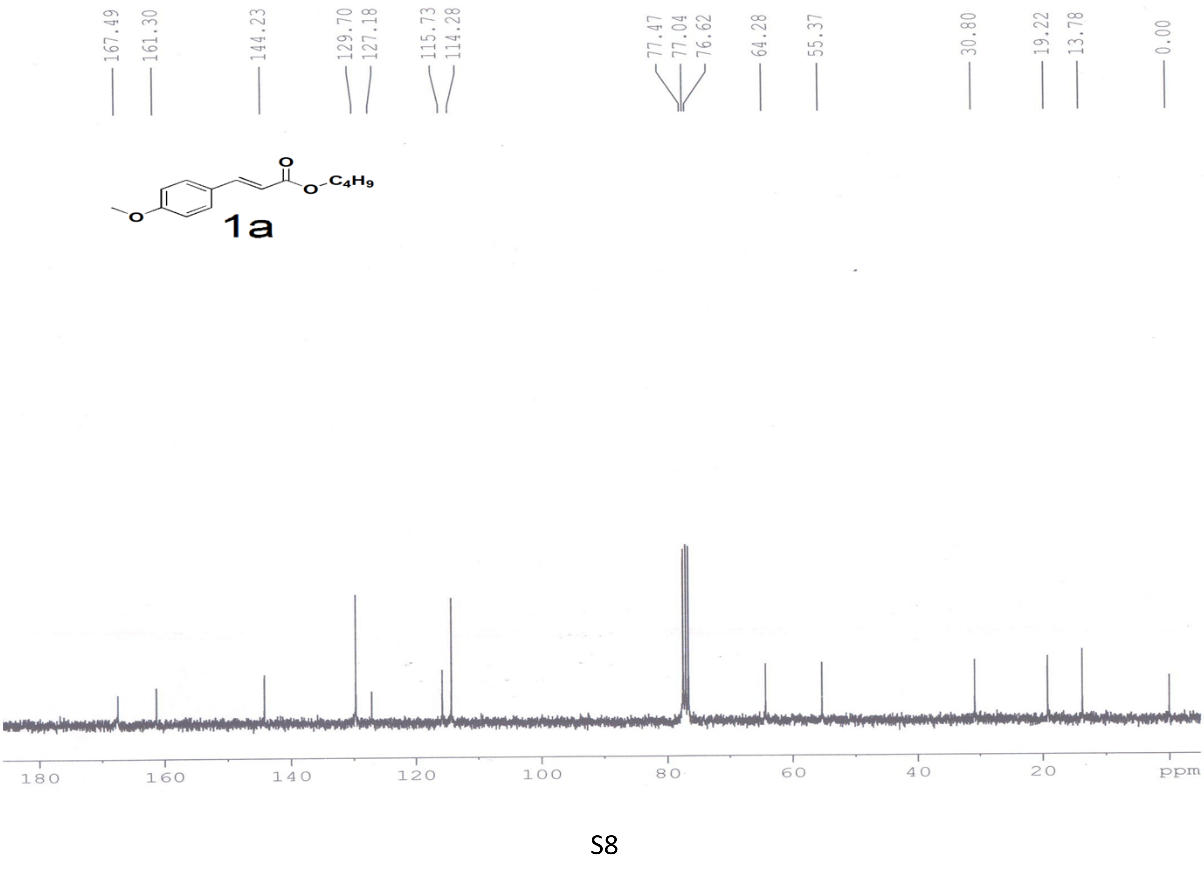
^{1}H and ^{13}C NMR spectra of 1a





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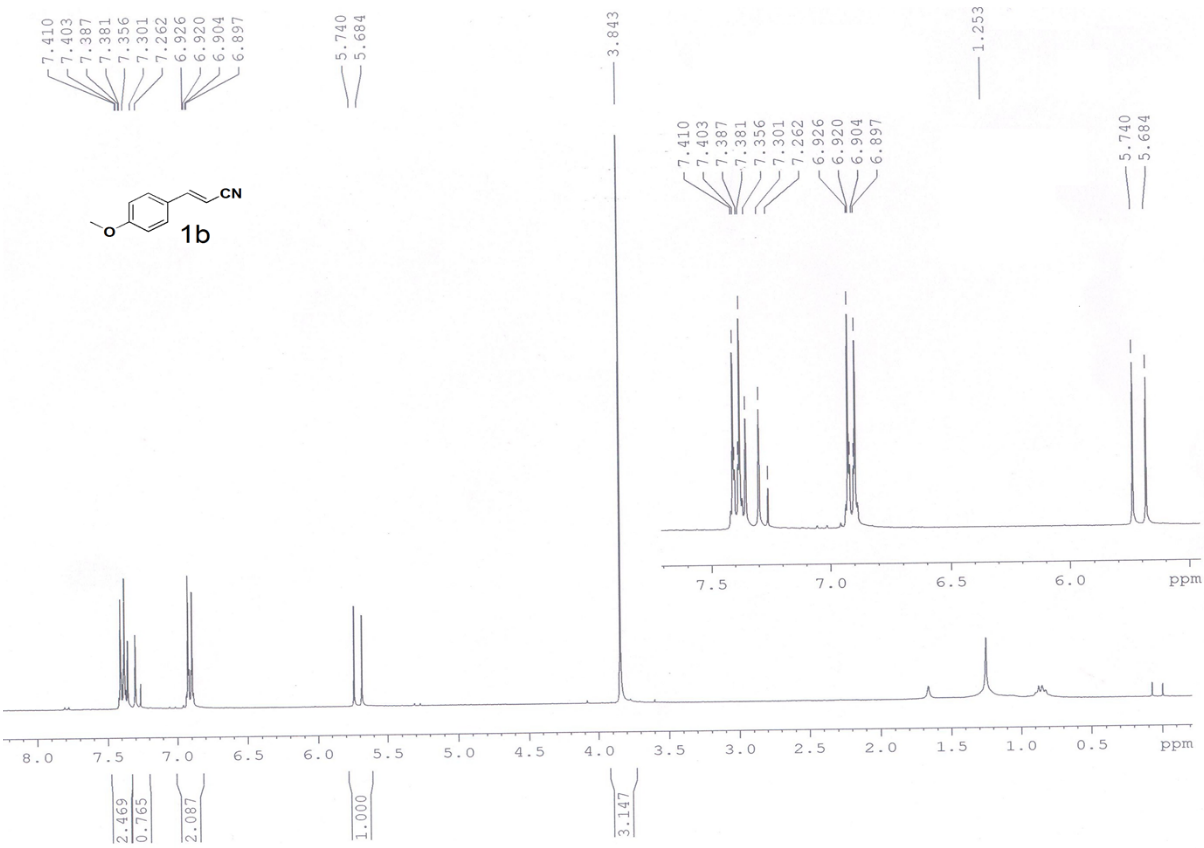

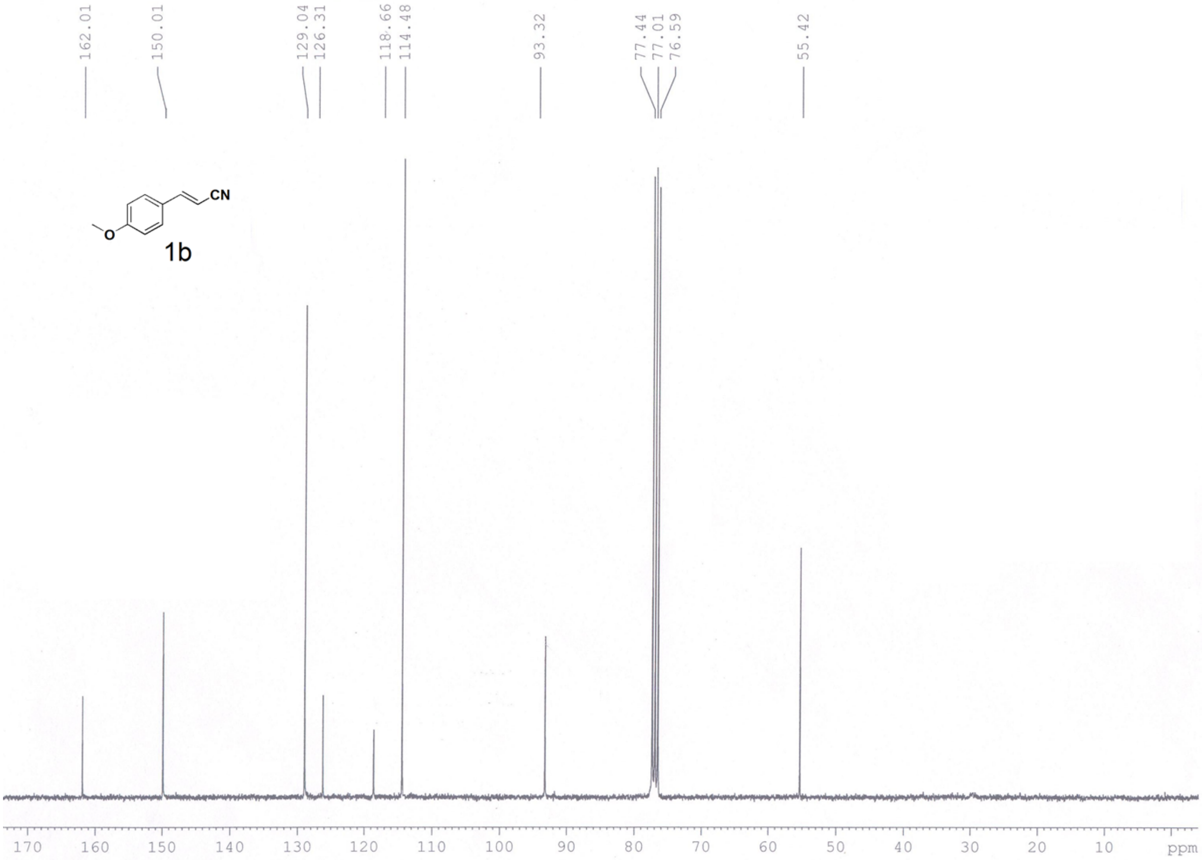

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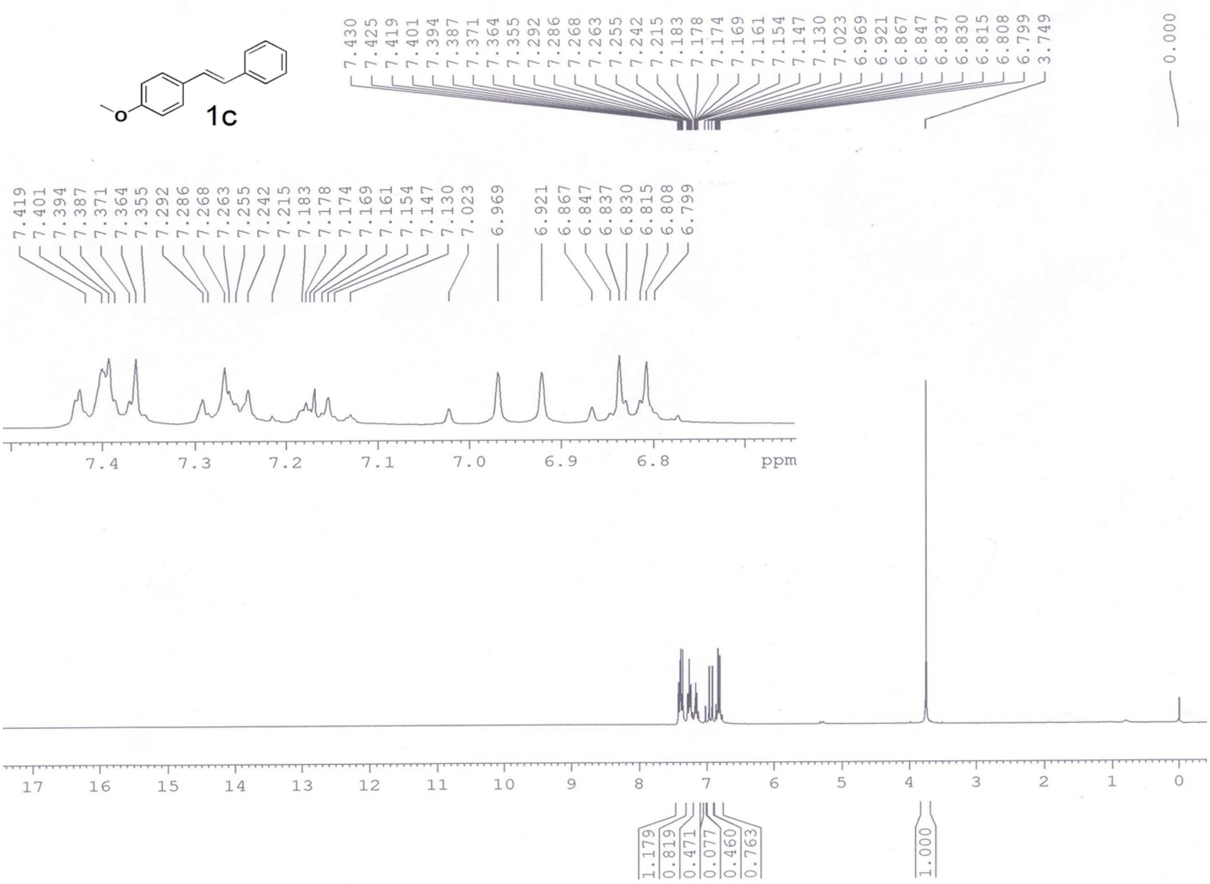

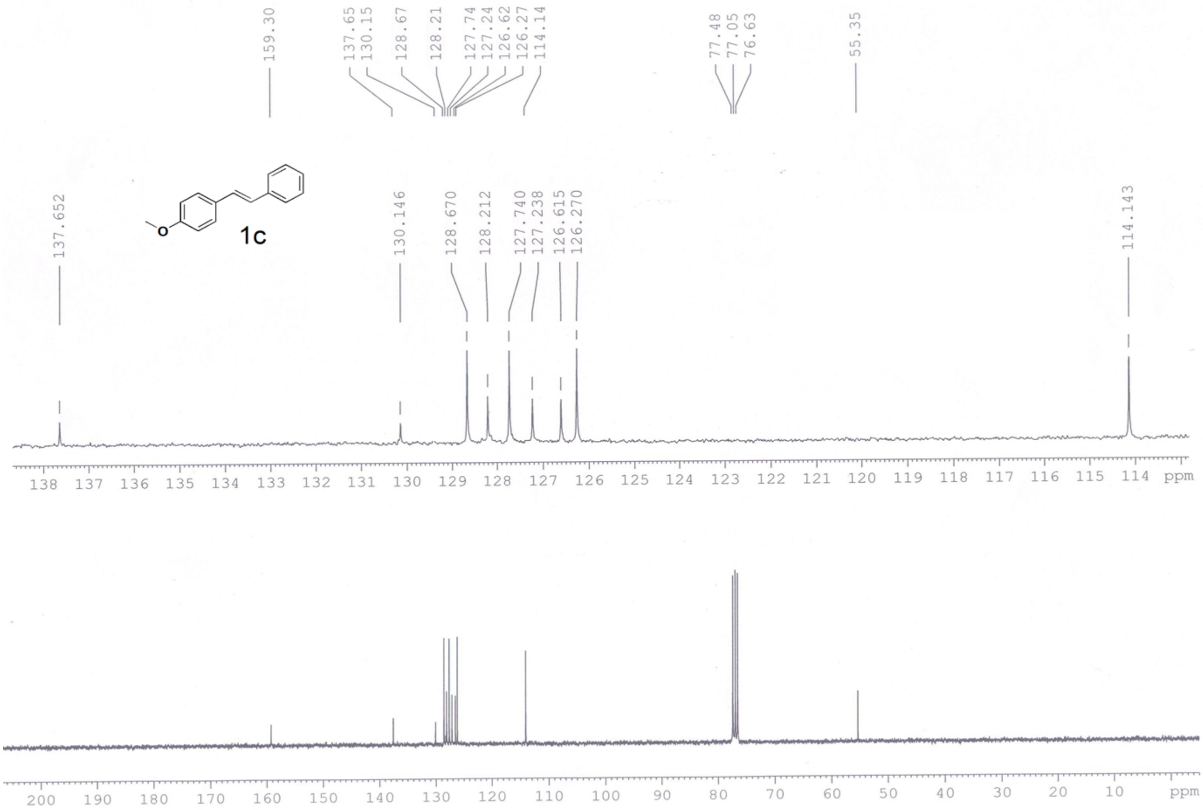

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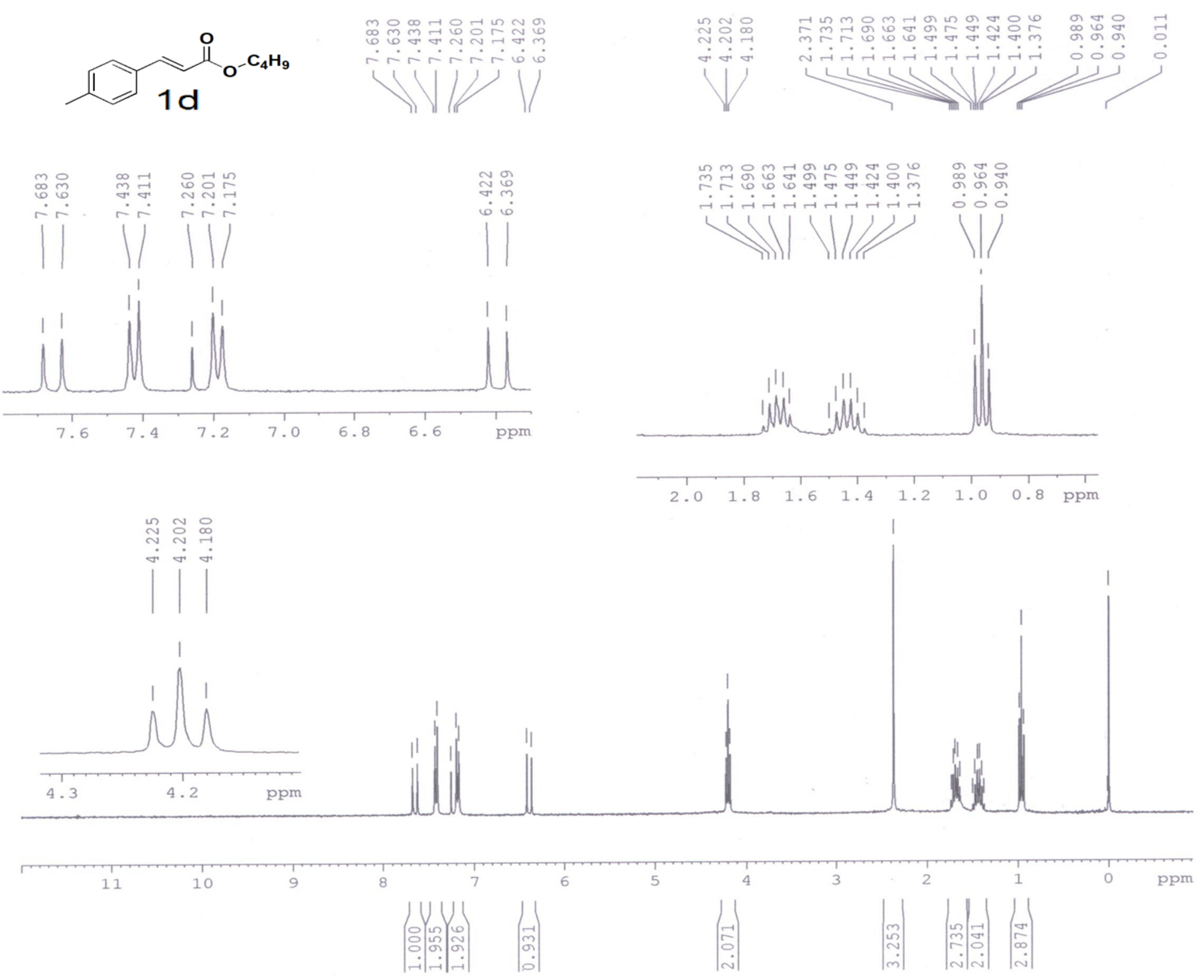

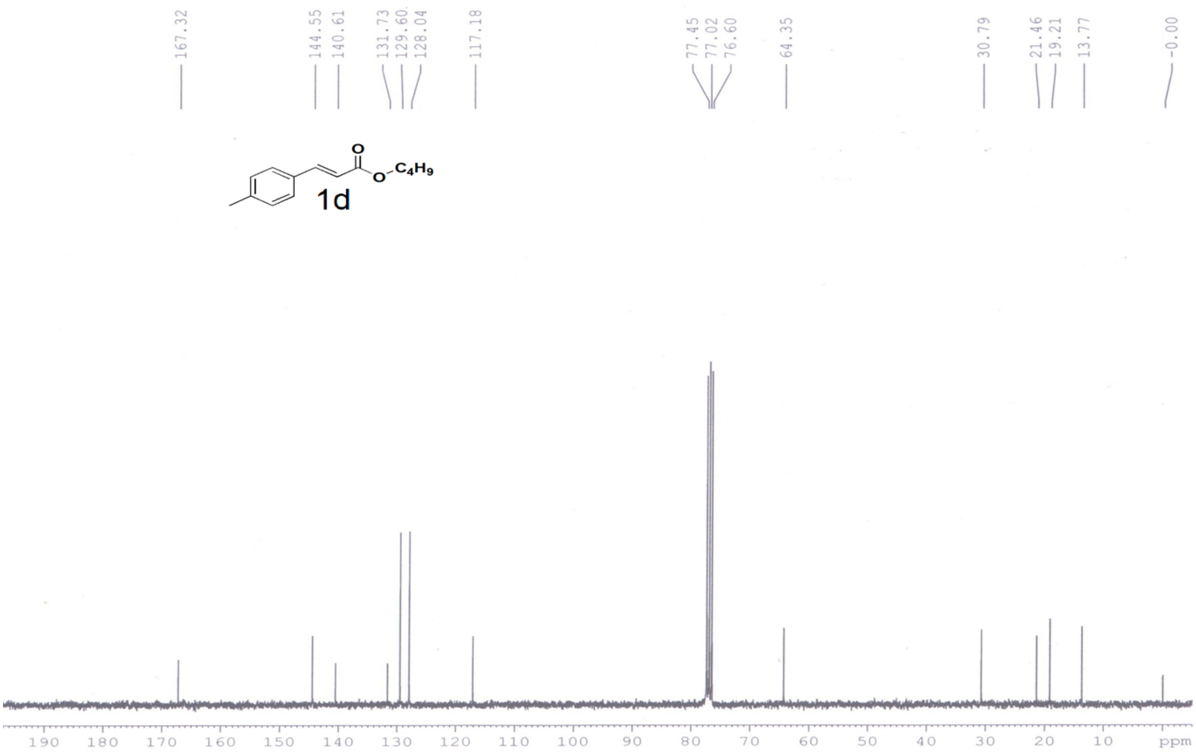

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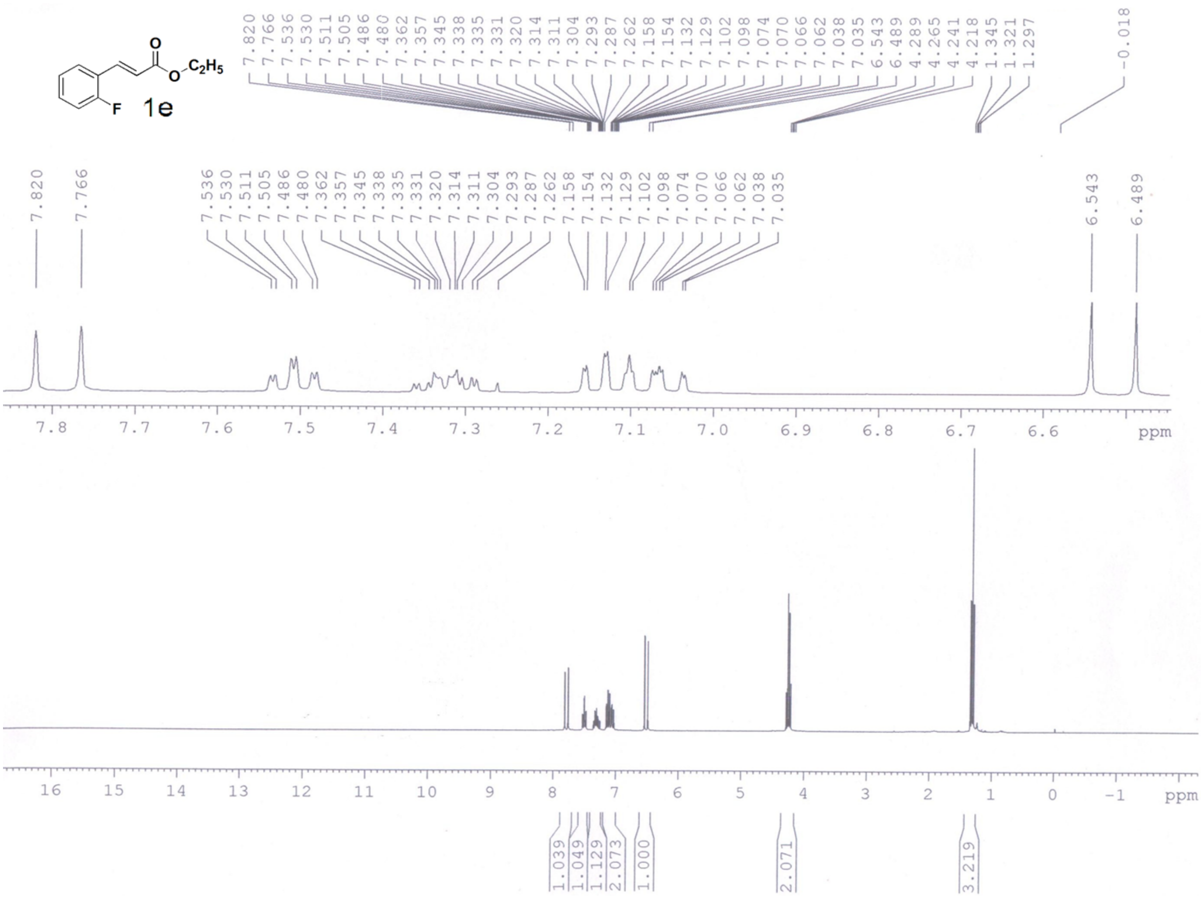

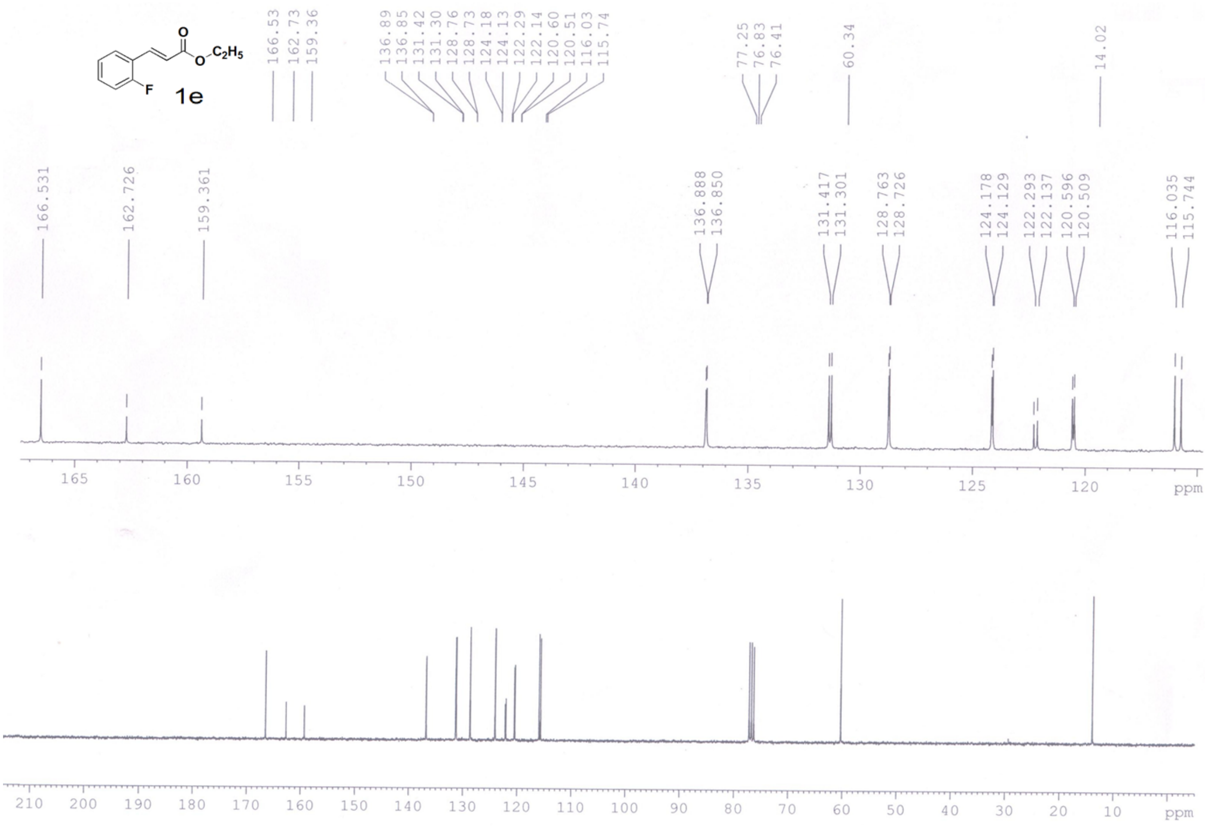

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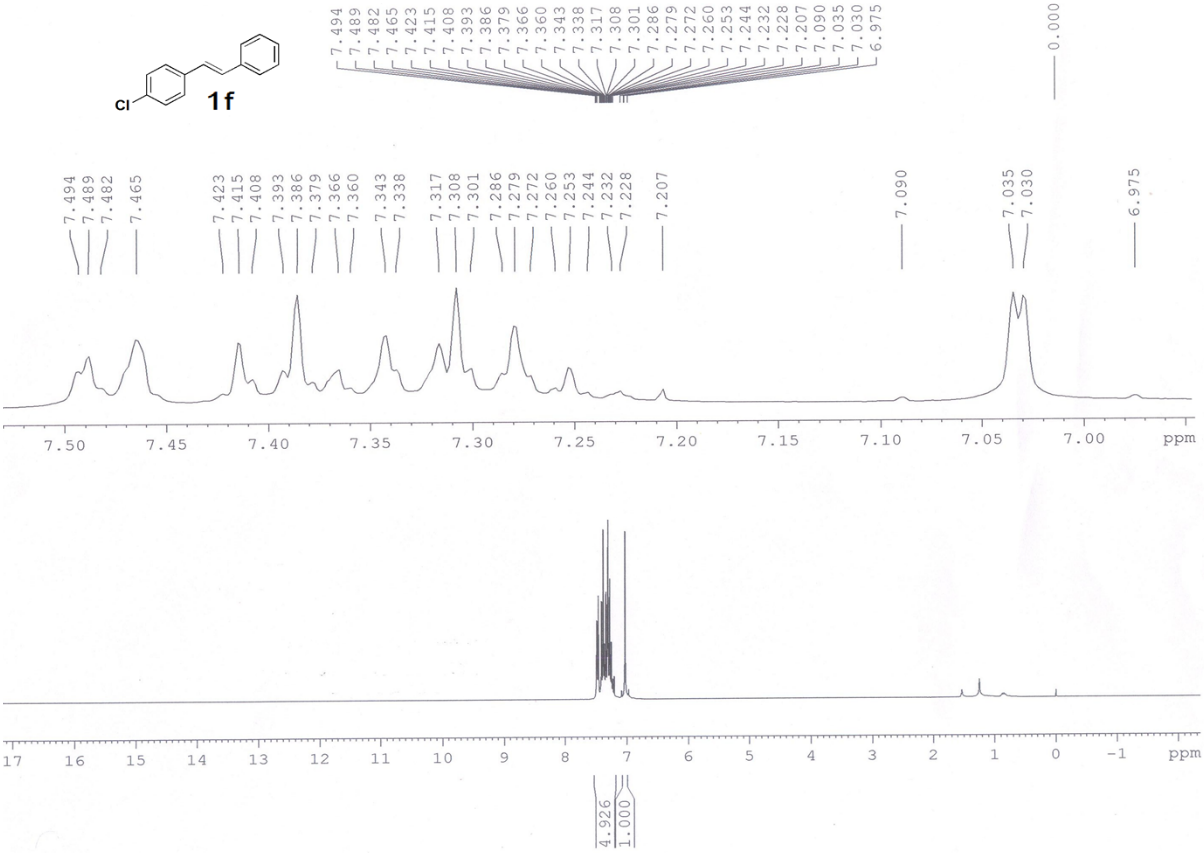

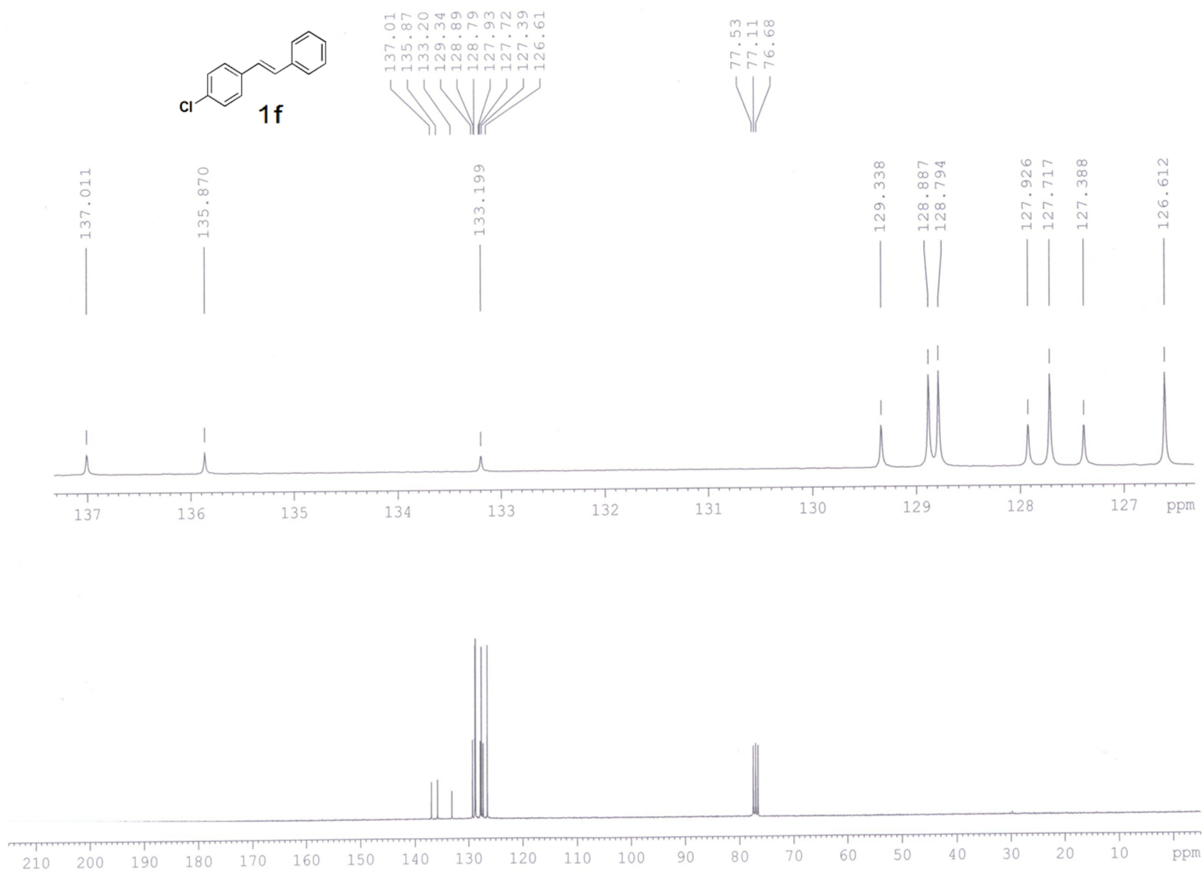

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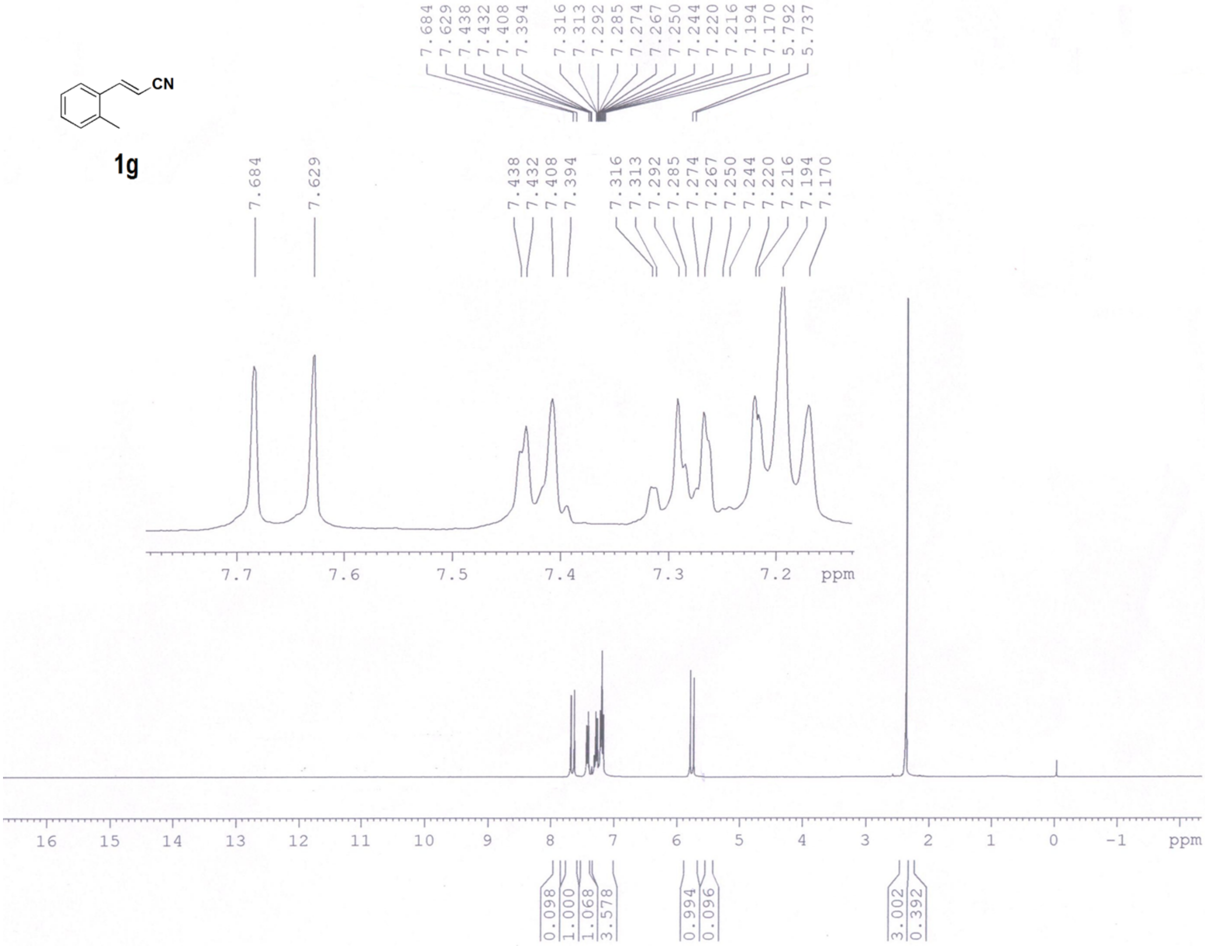

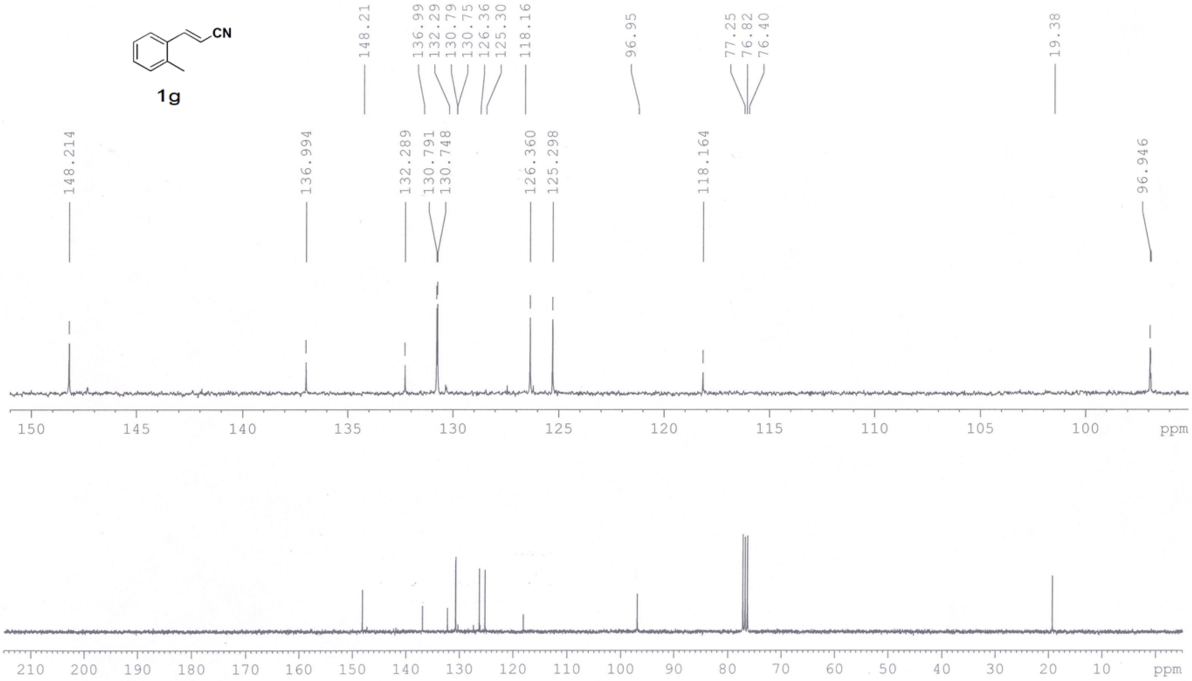

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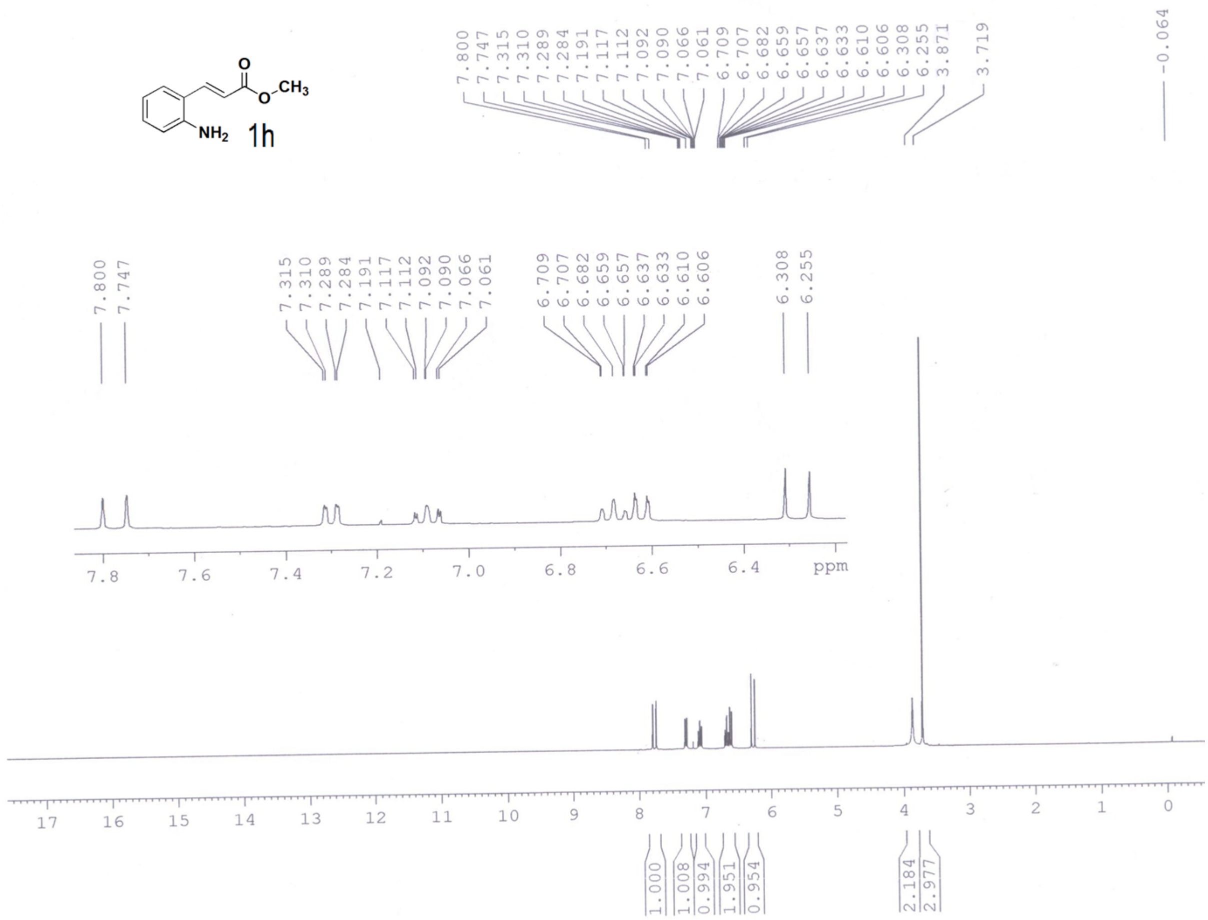

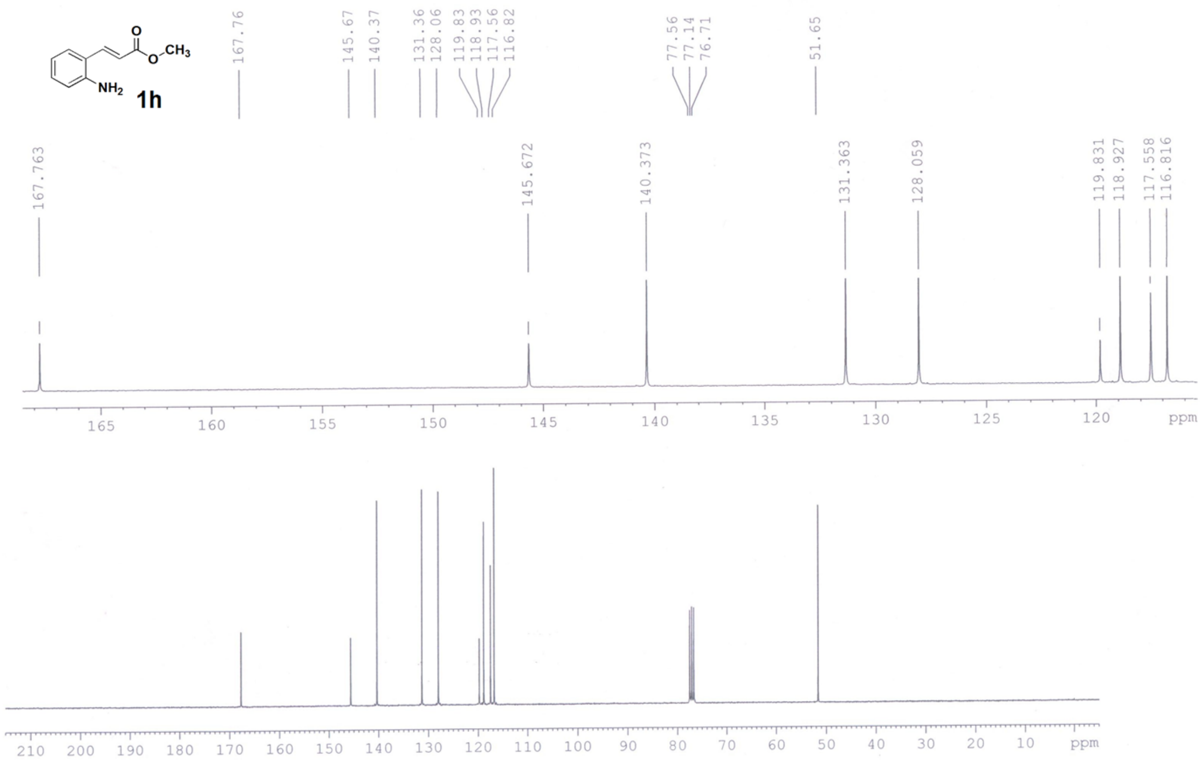

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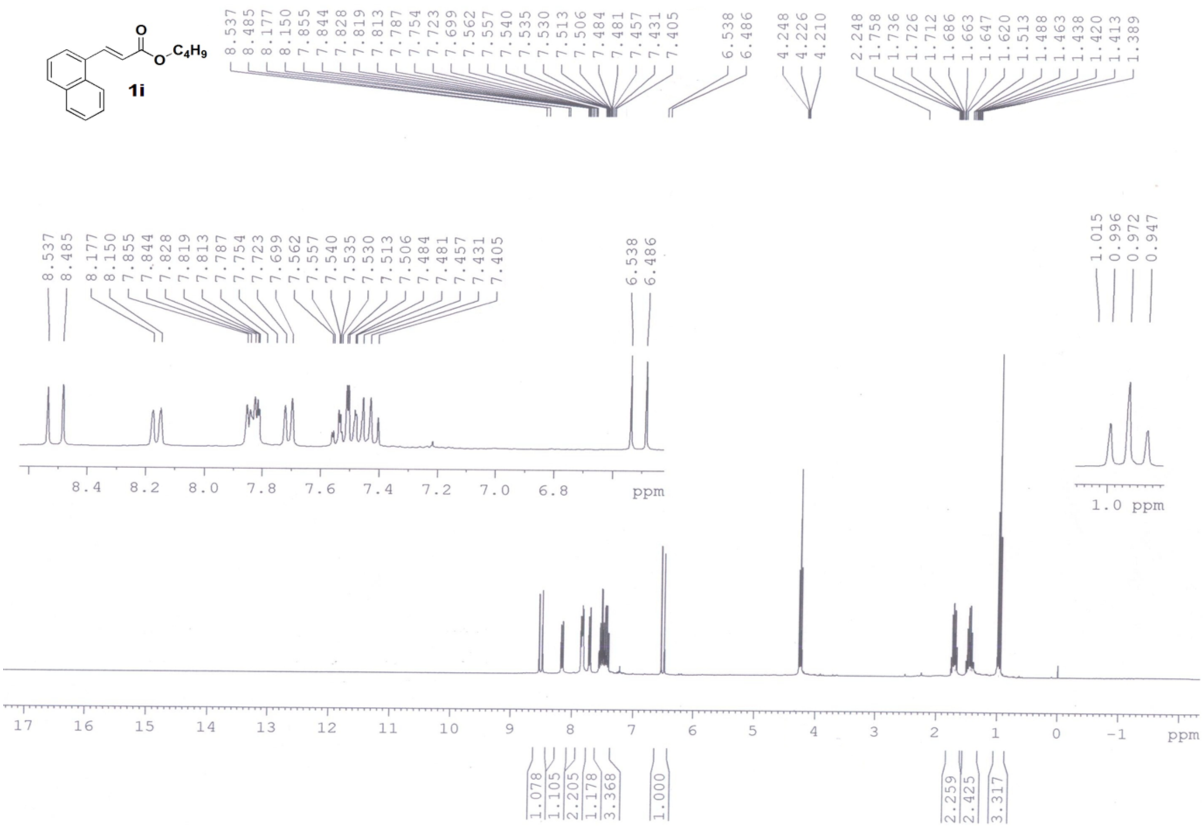

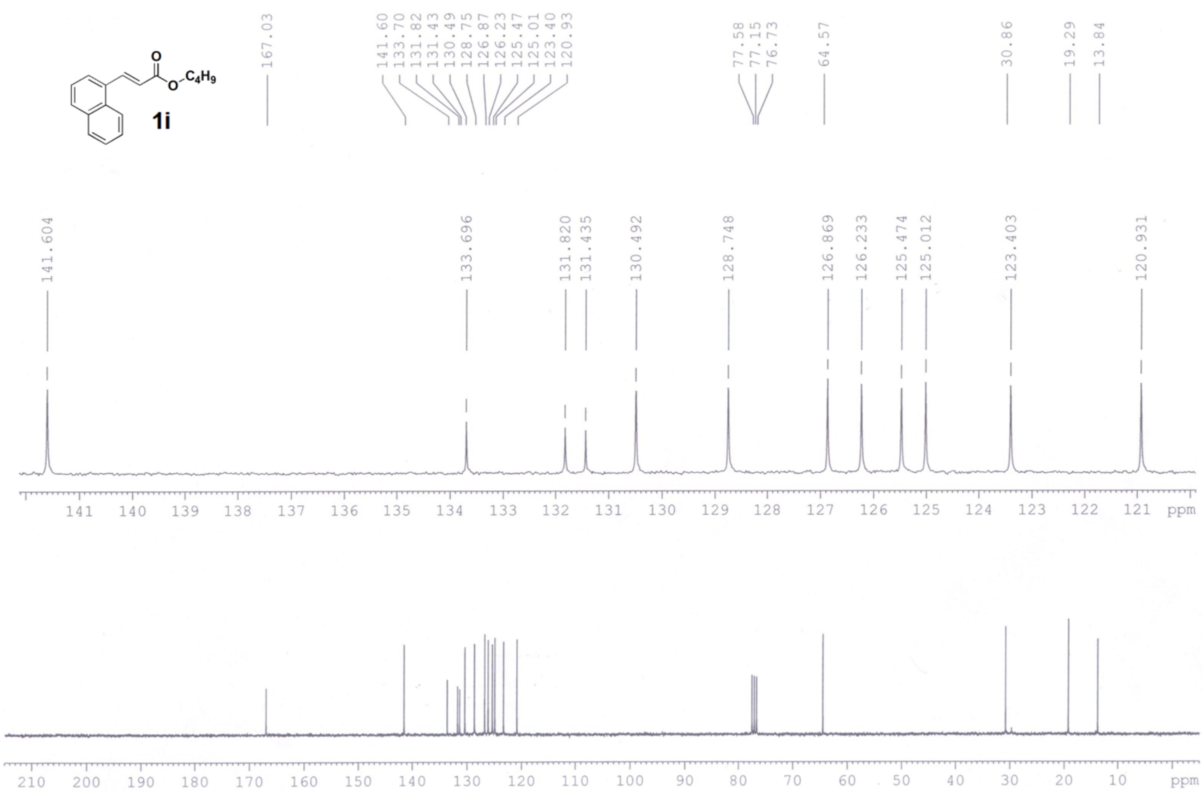

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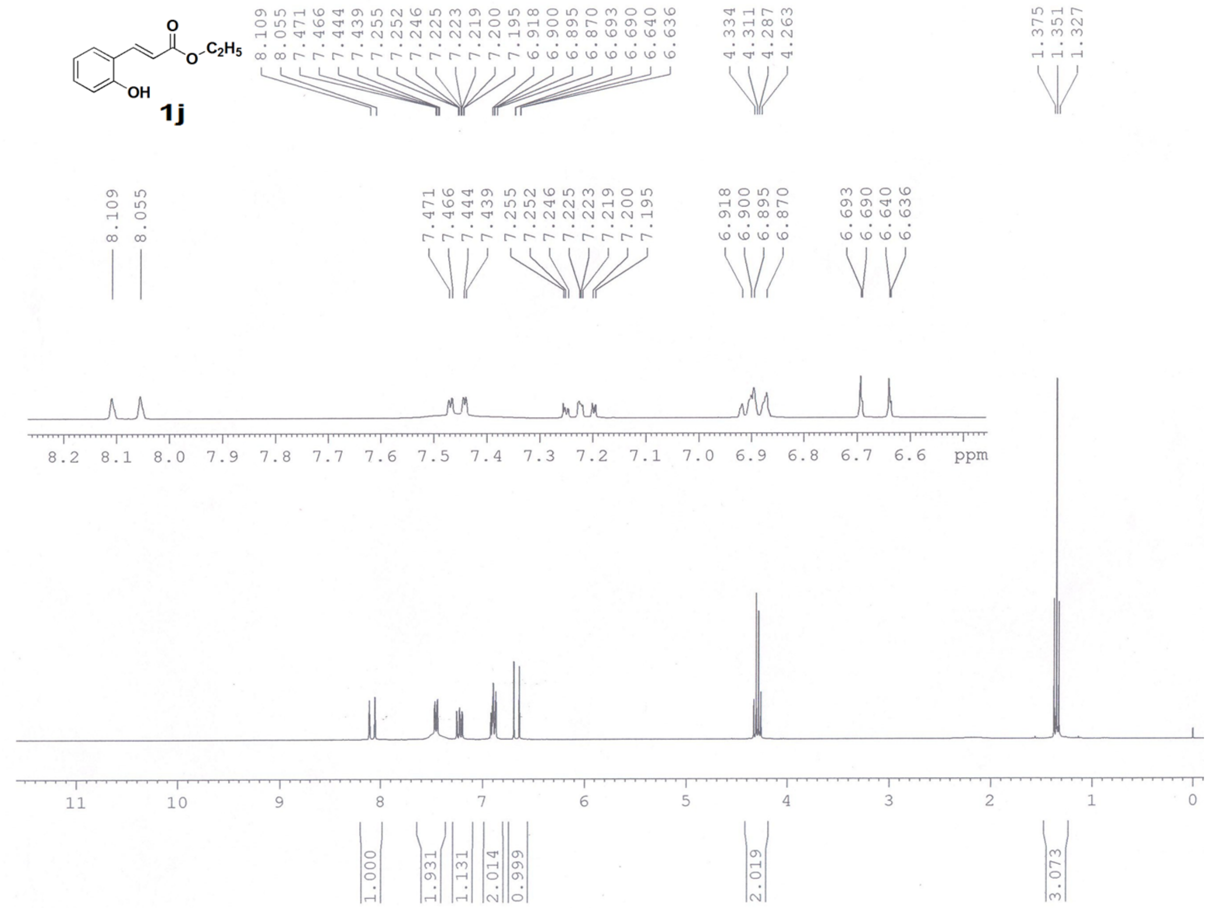
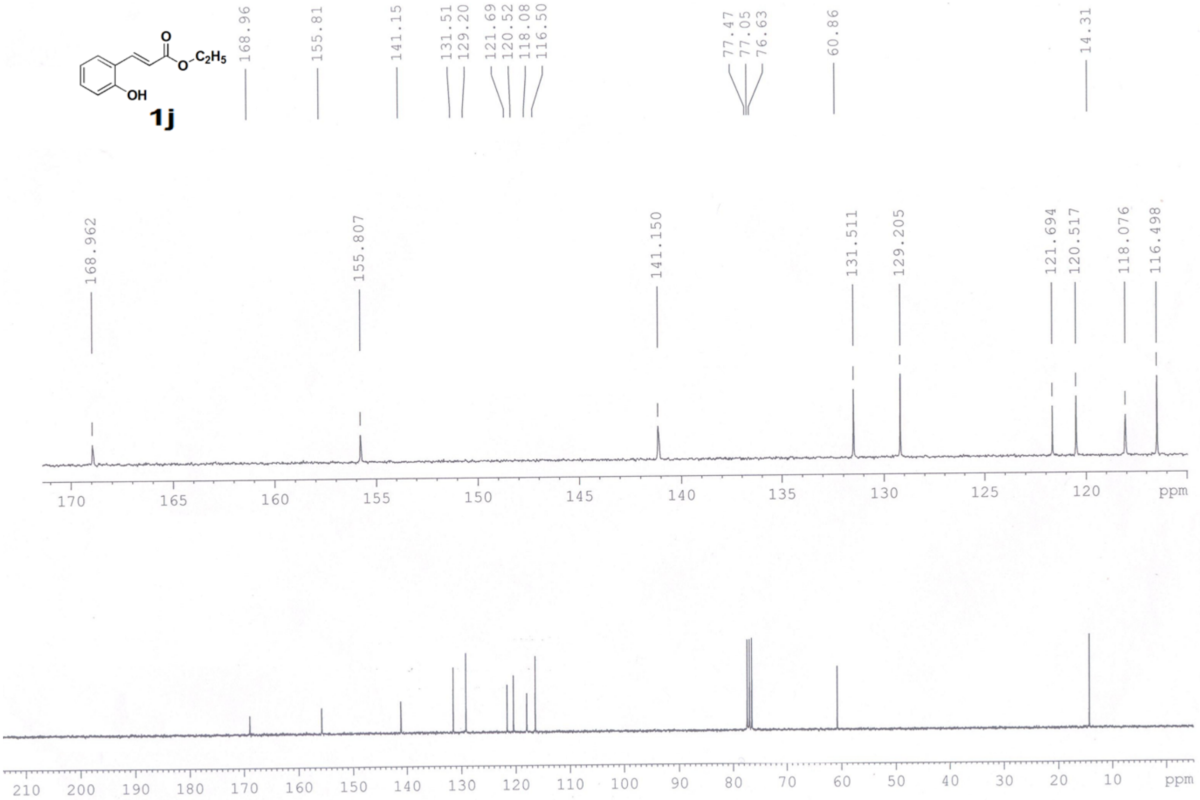
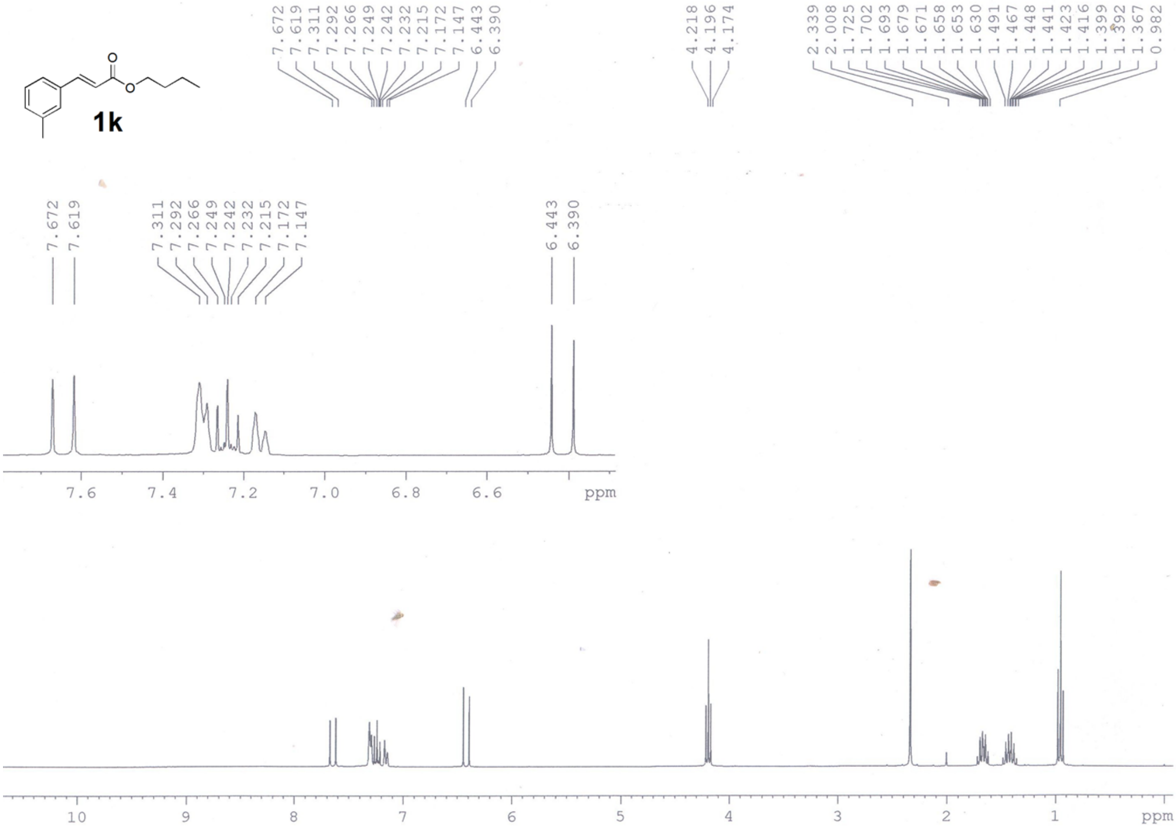
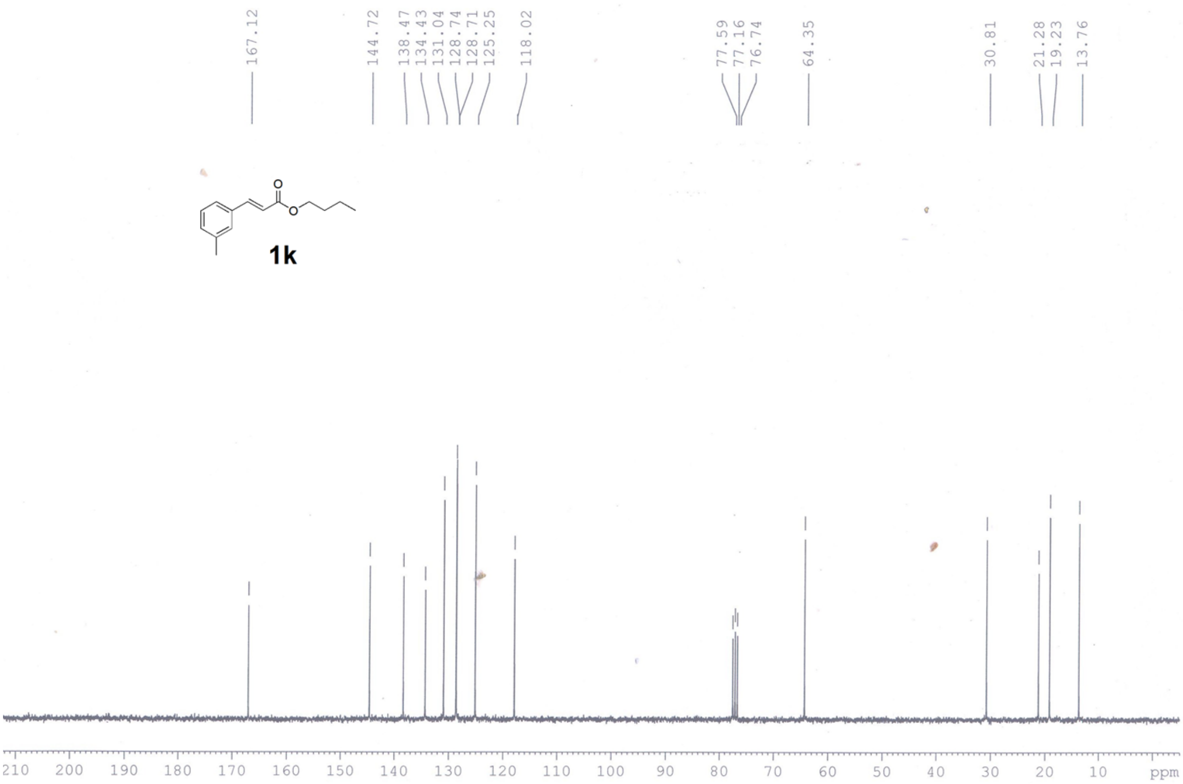


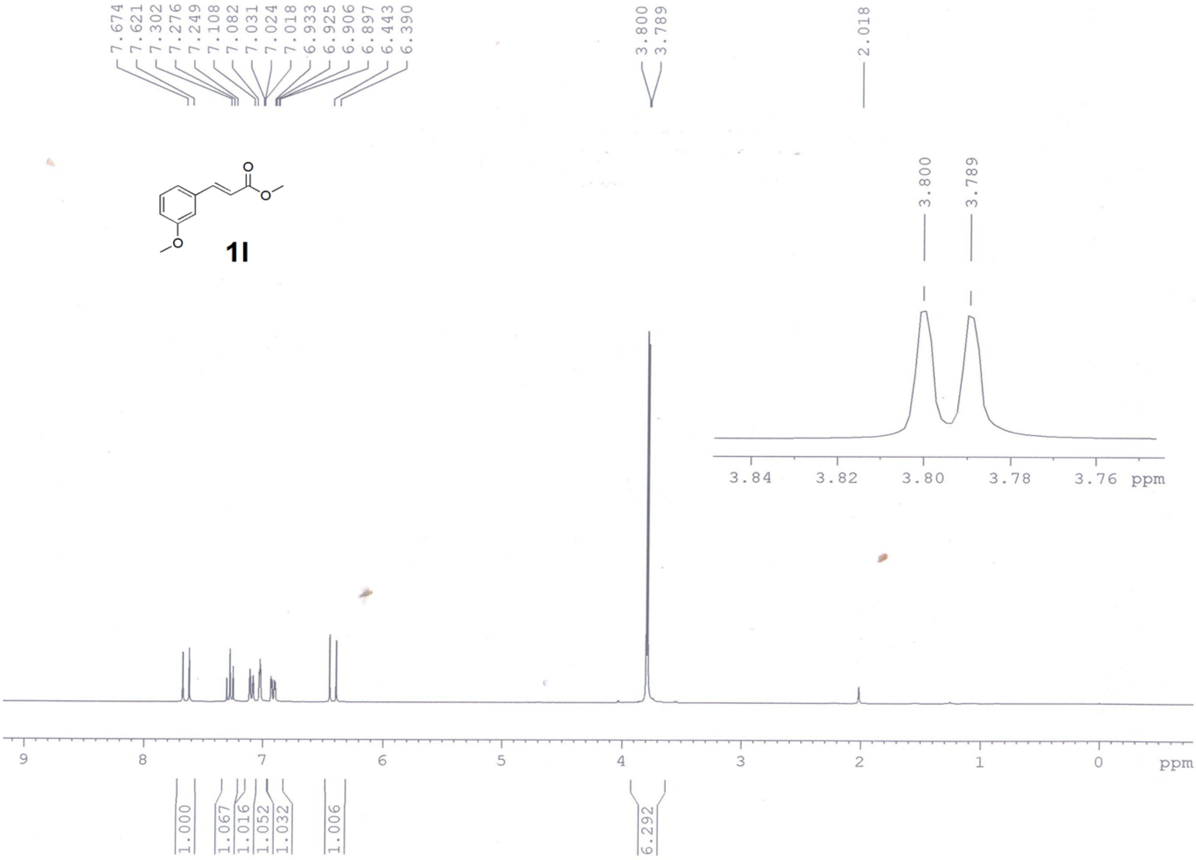


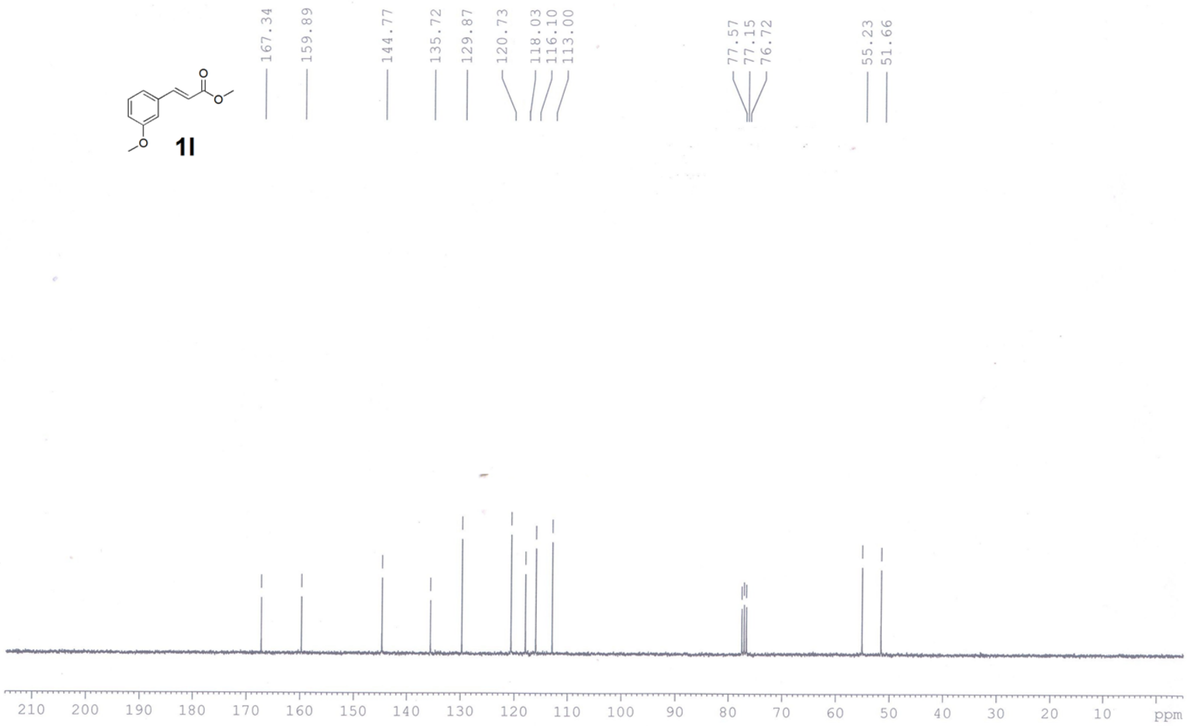
^{1}H and ^{13}C NMR spectra of 1k



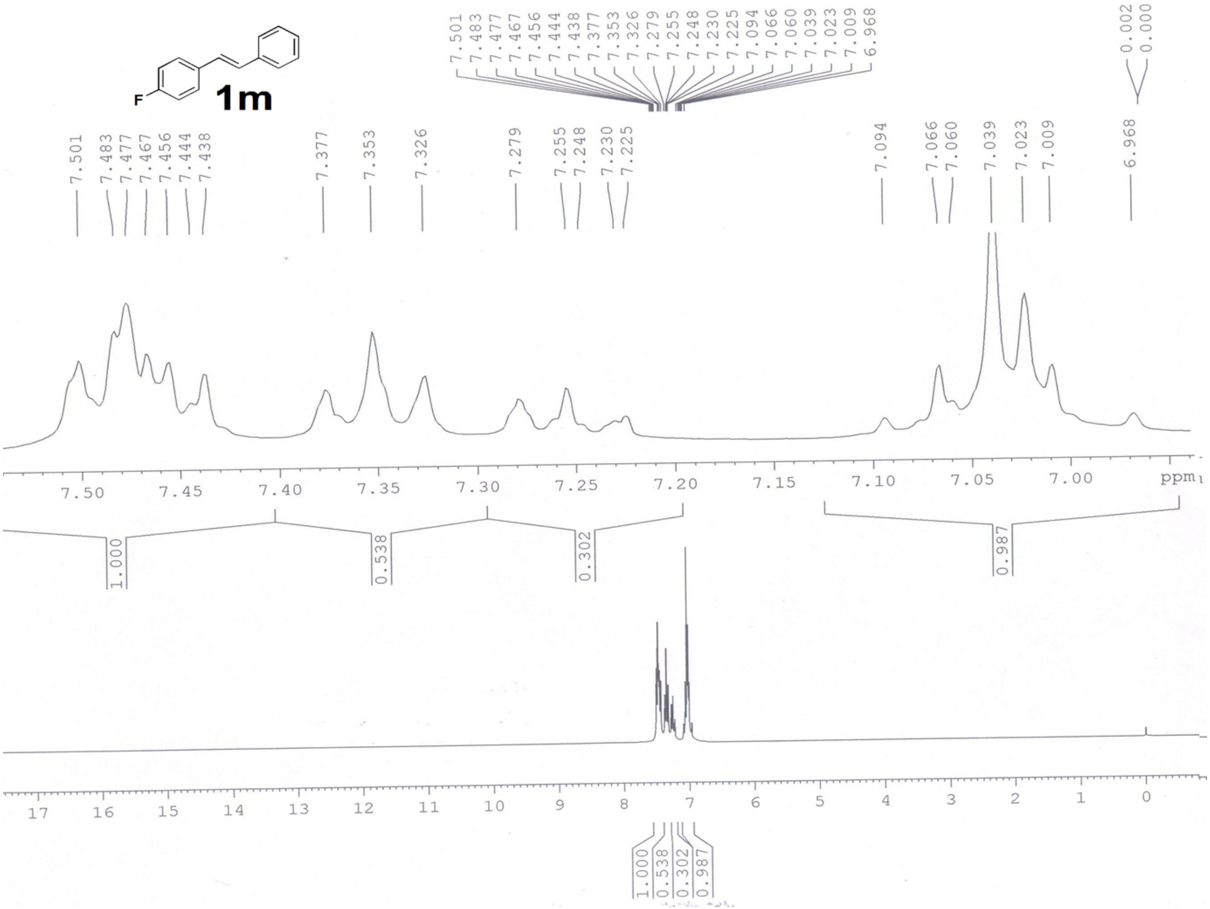


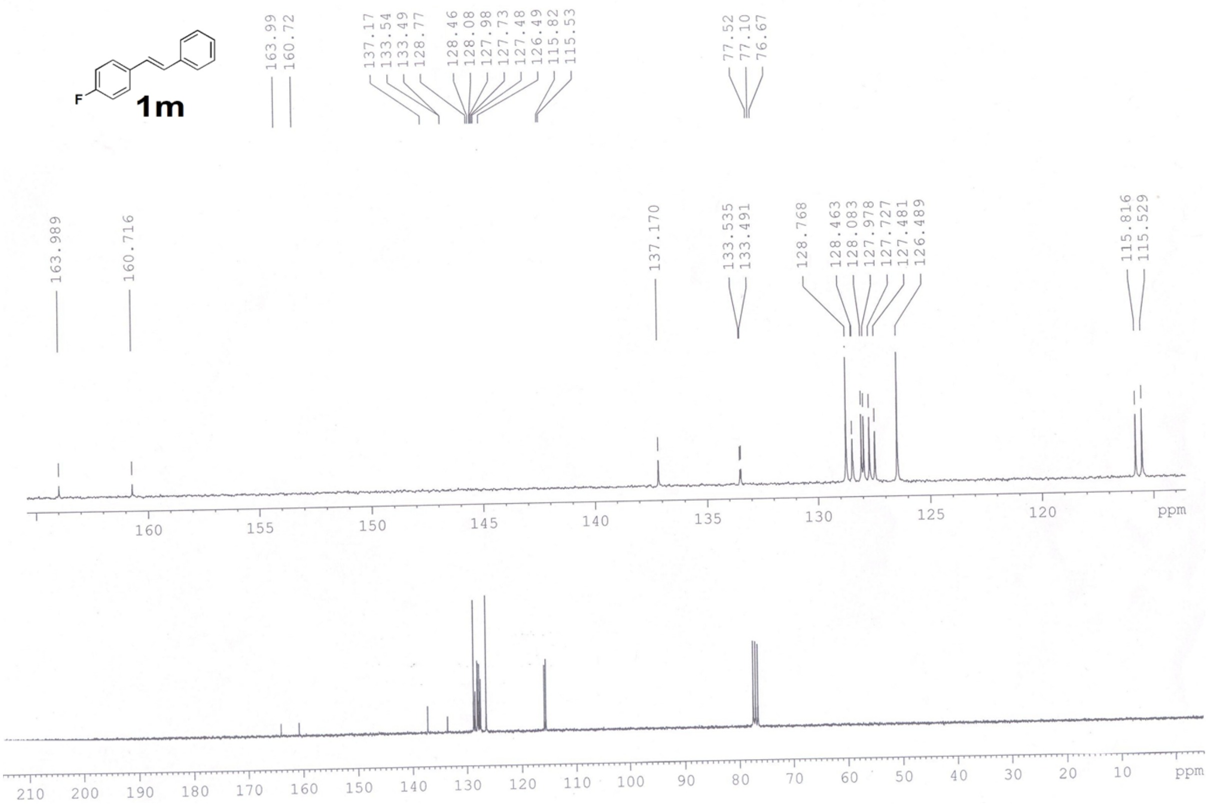
^{1}H and ^{13}C NMR spectra of 1l



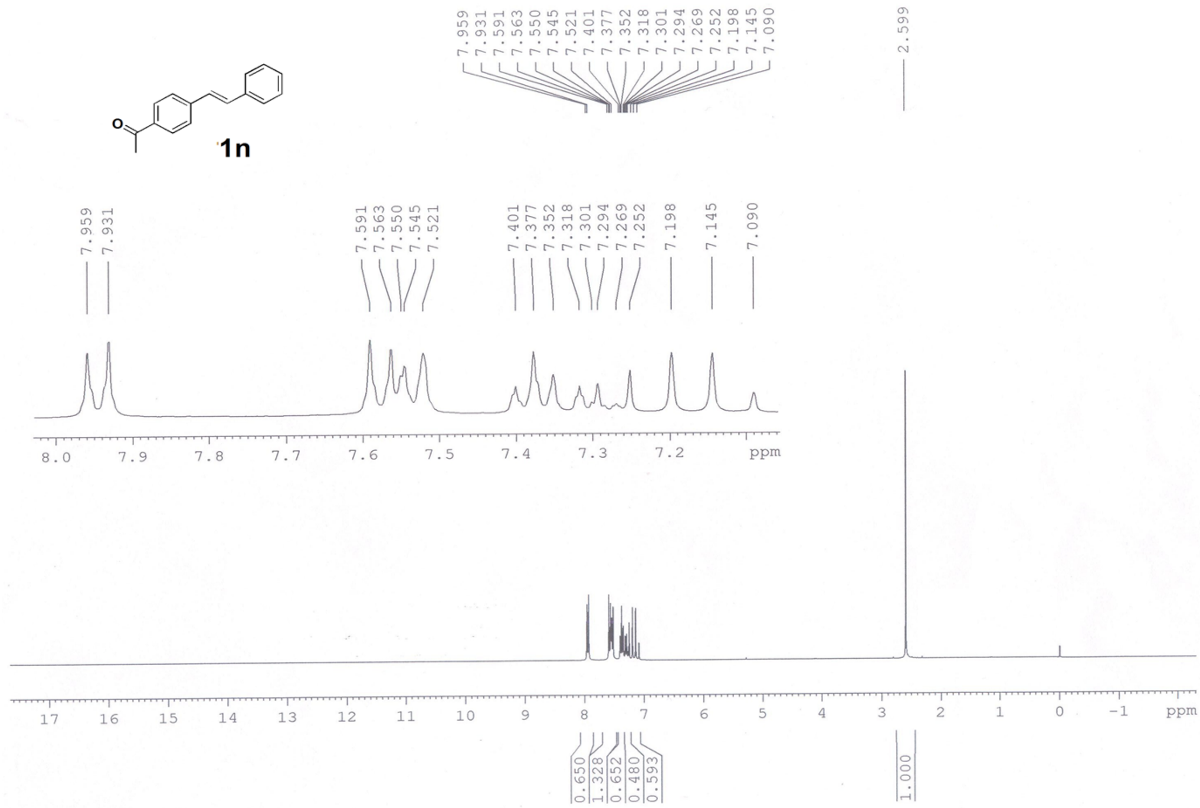


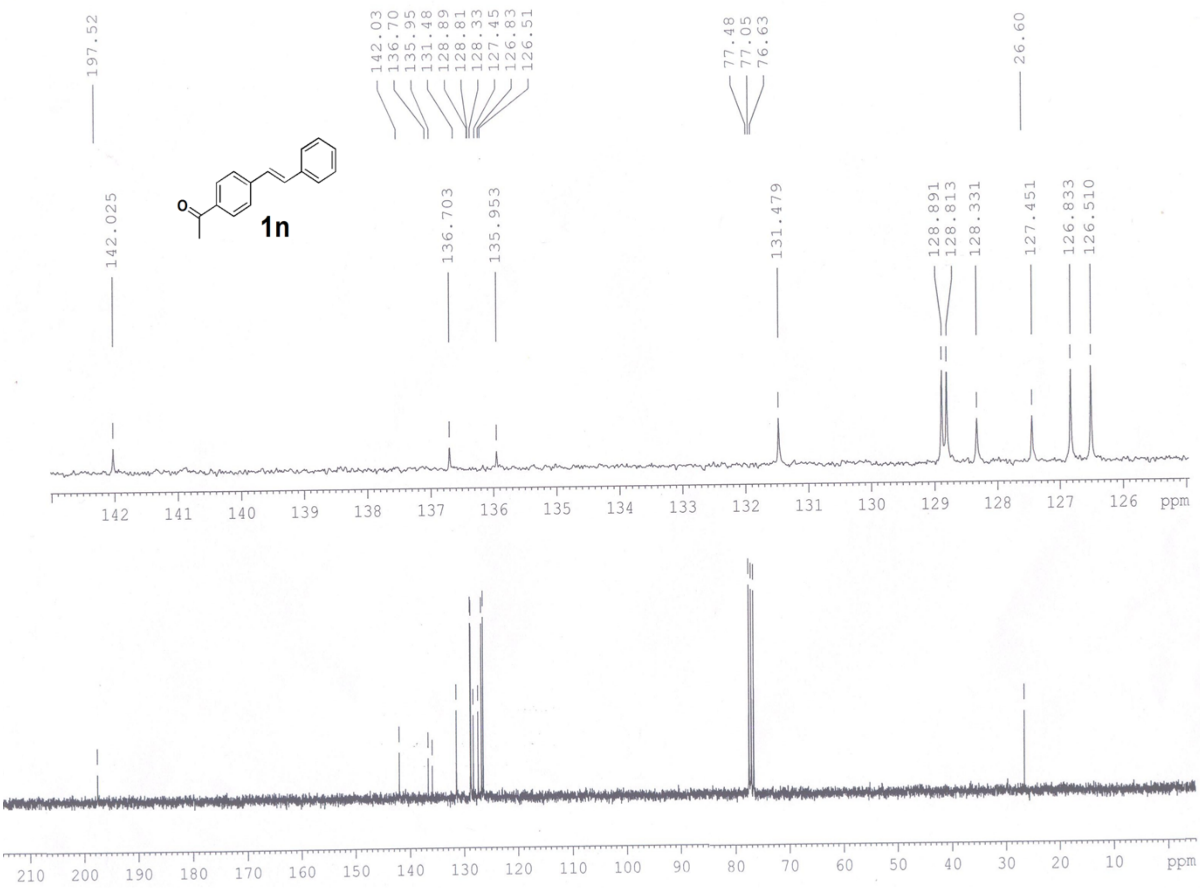
^{1}H and ^{13}C NMR spectra of 1m



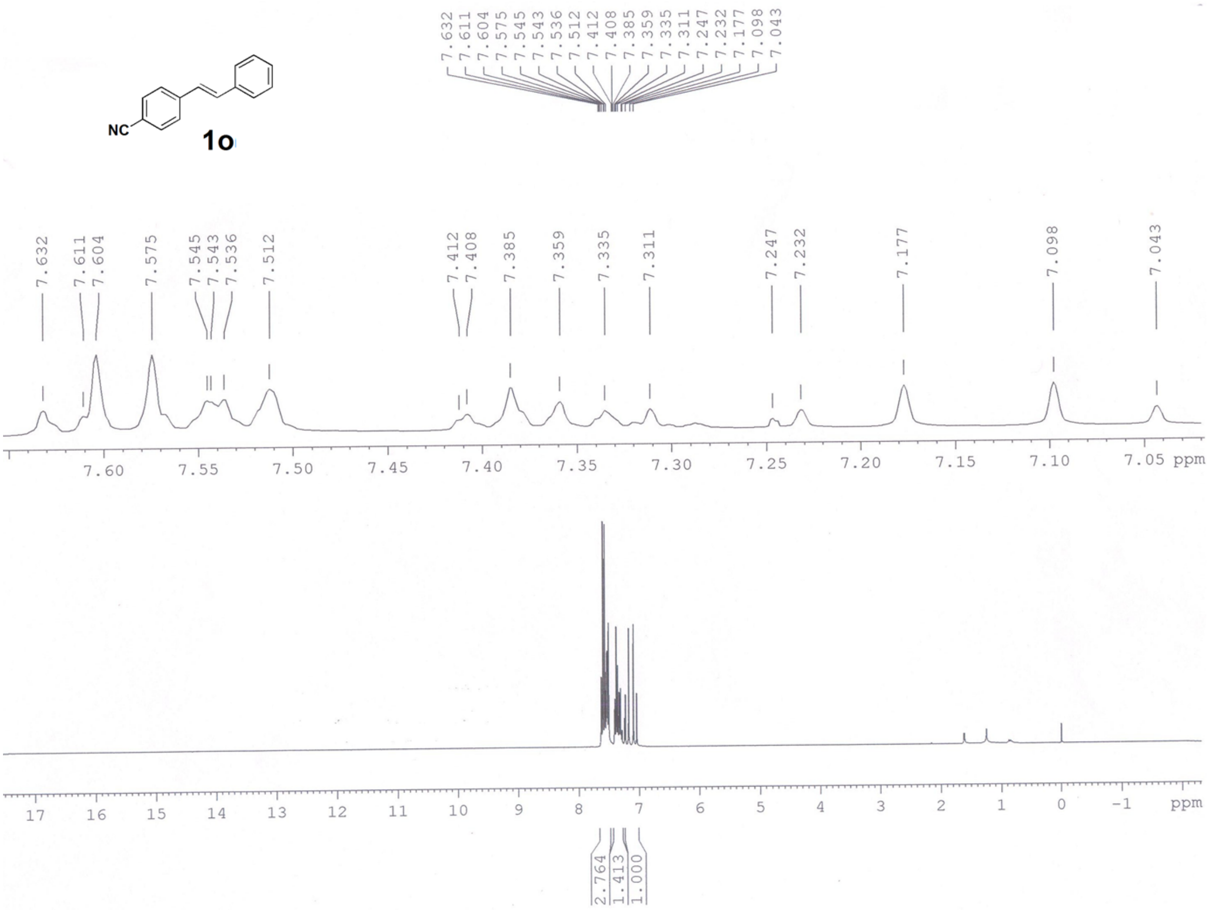


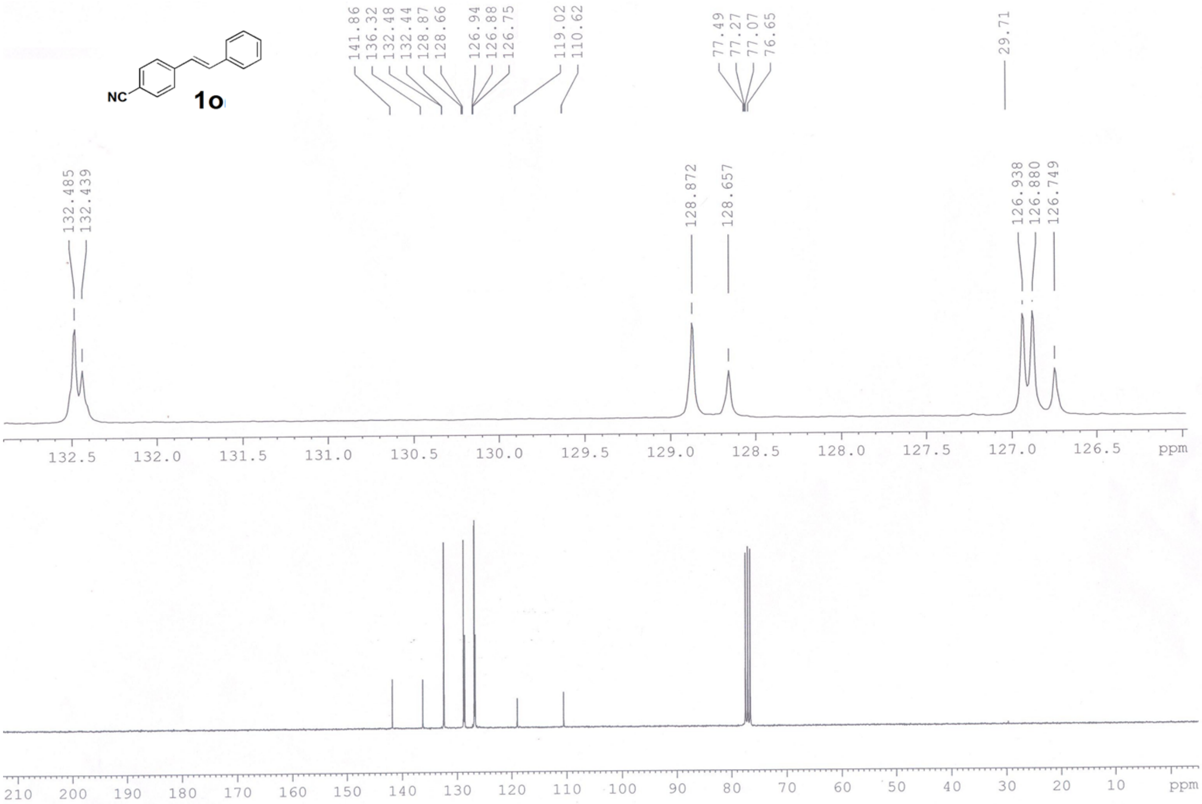
^{1}H and ^{13}C NMR spectra of 1n



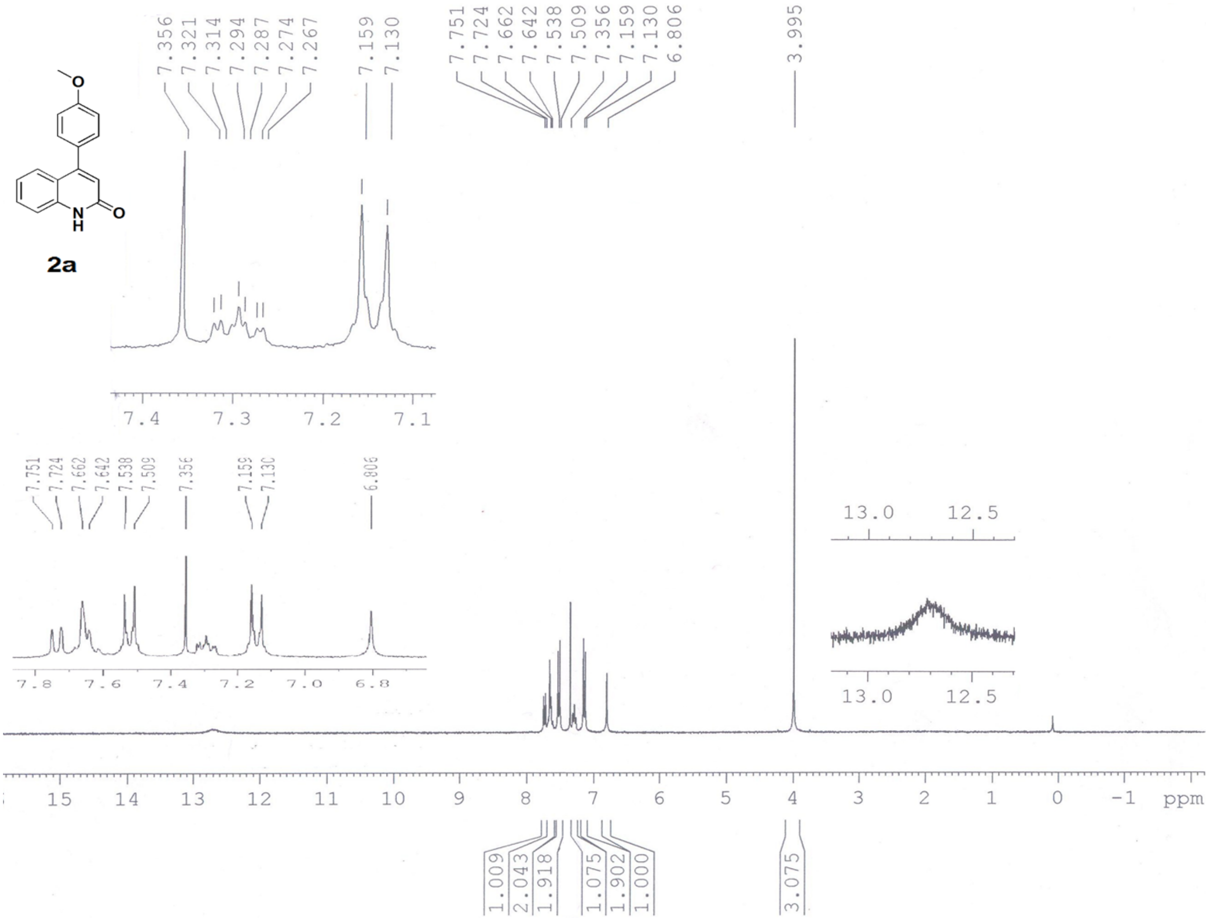


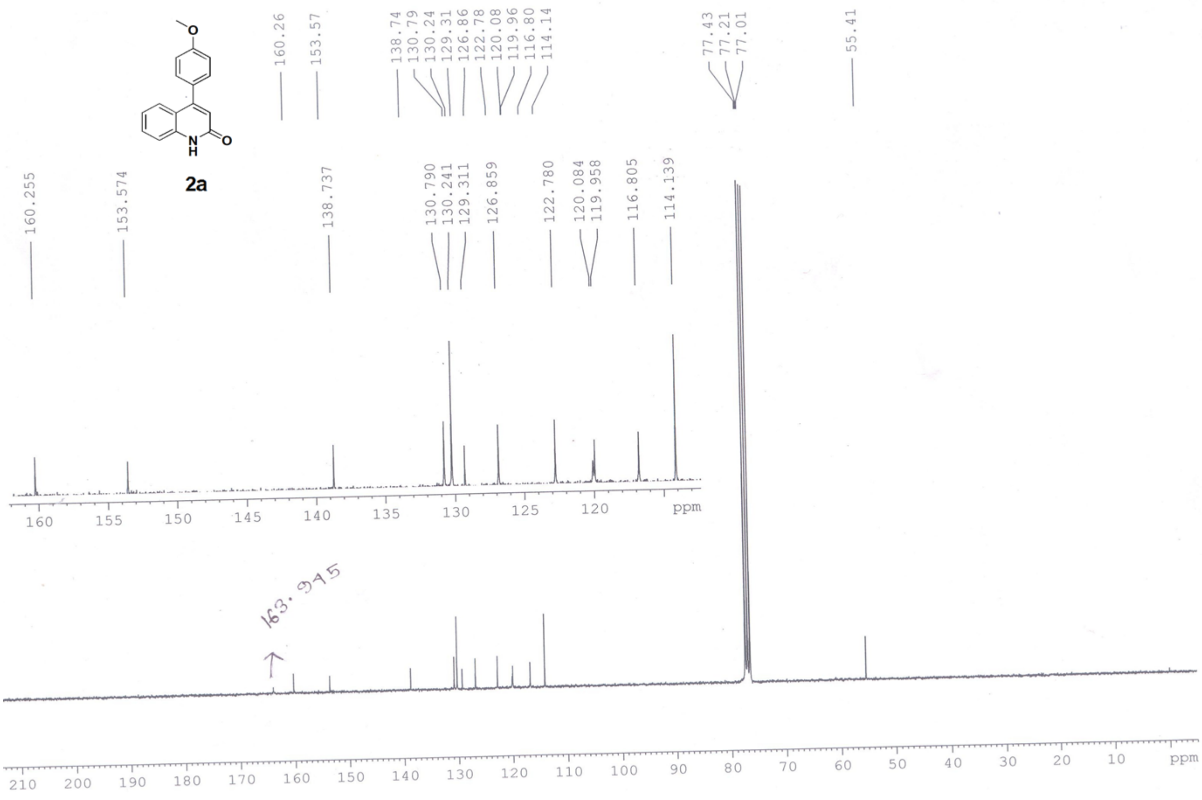
^{1}H and ^{13}C NMR spectra of 1o



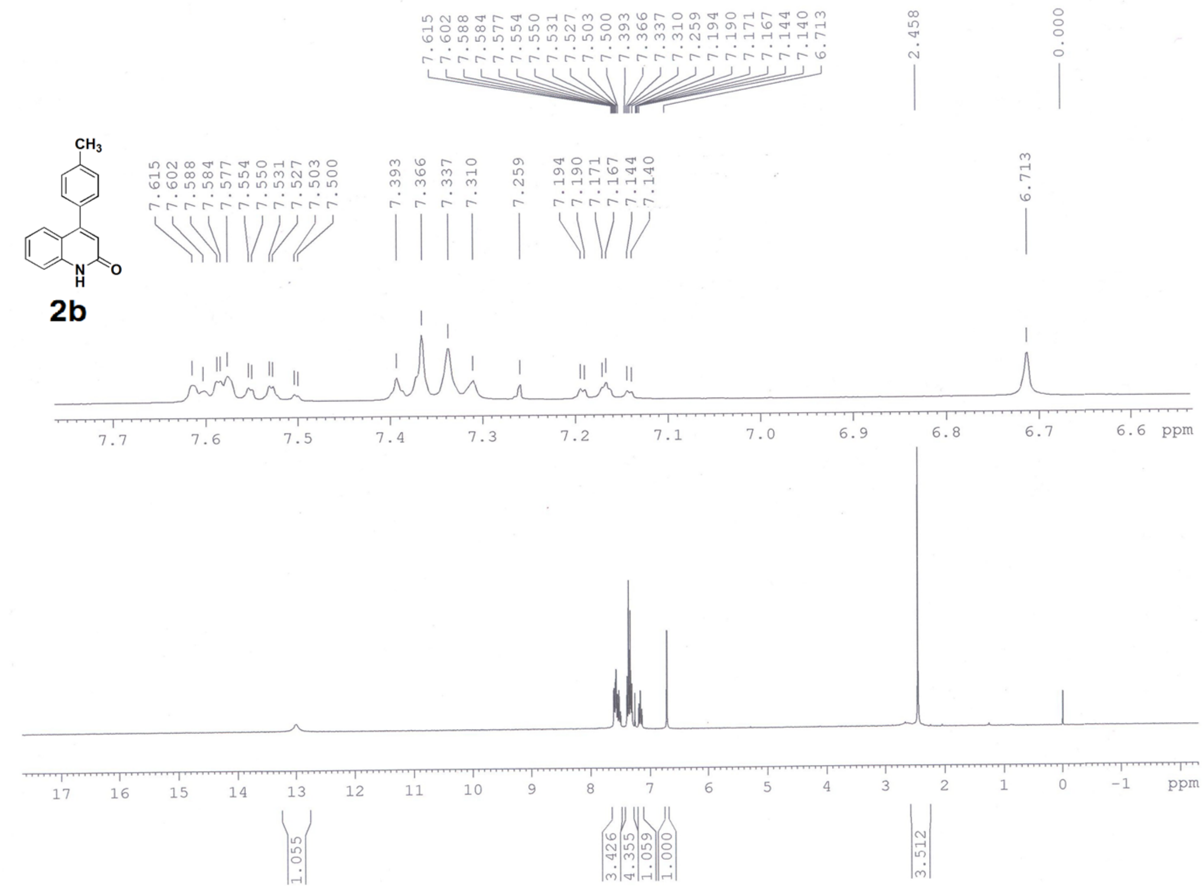


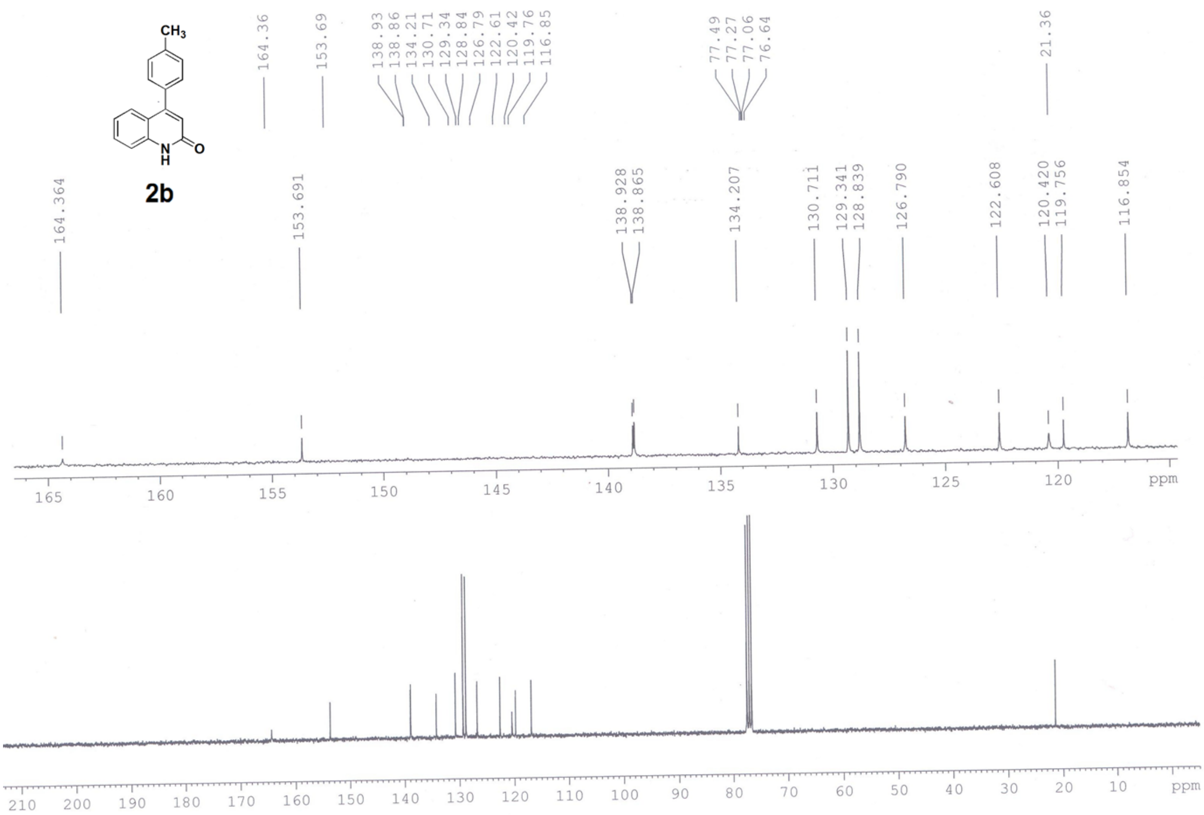
^{1}H and ^{13}C NMR spectra of 2a



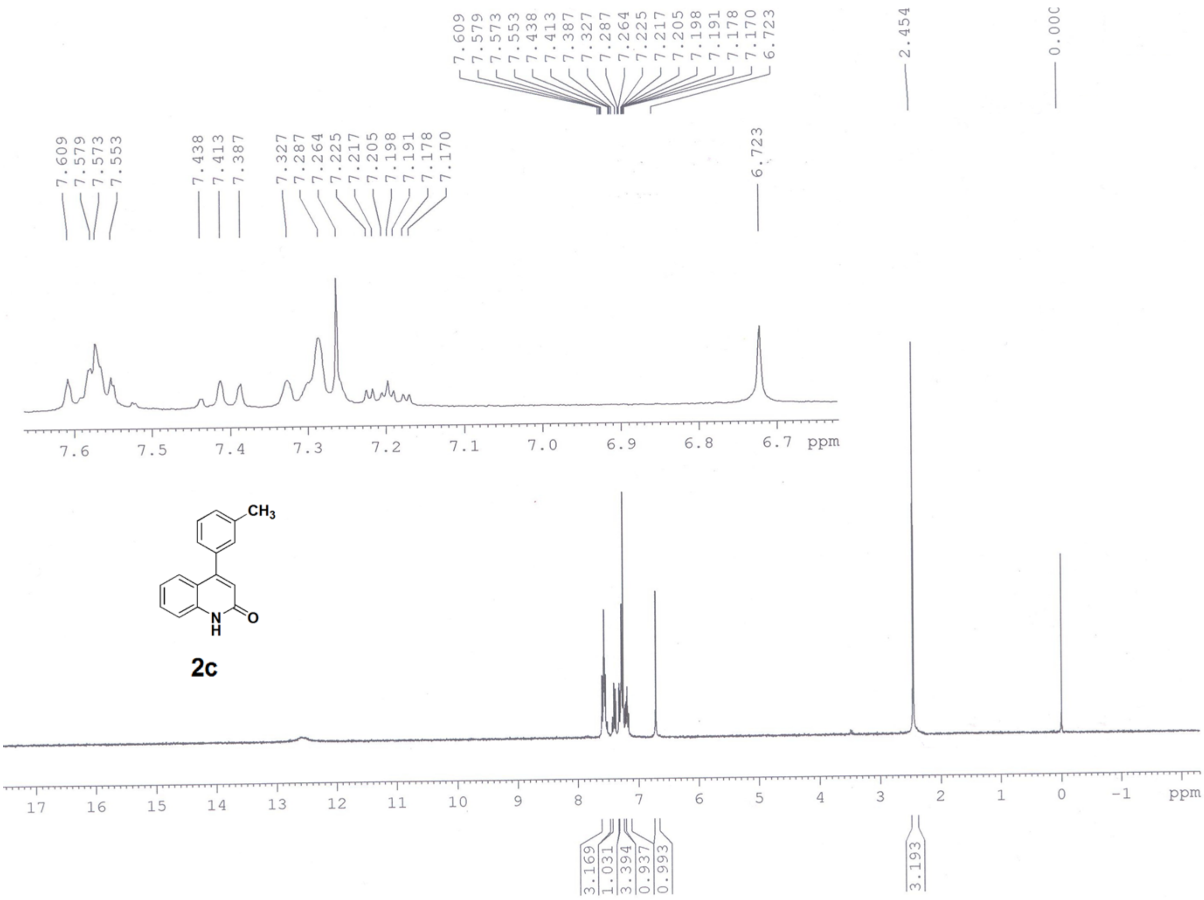


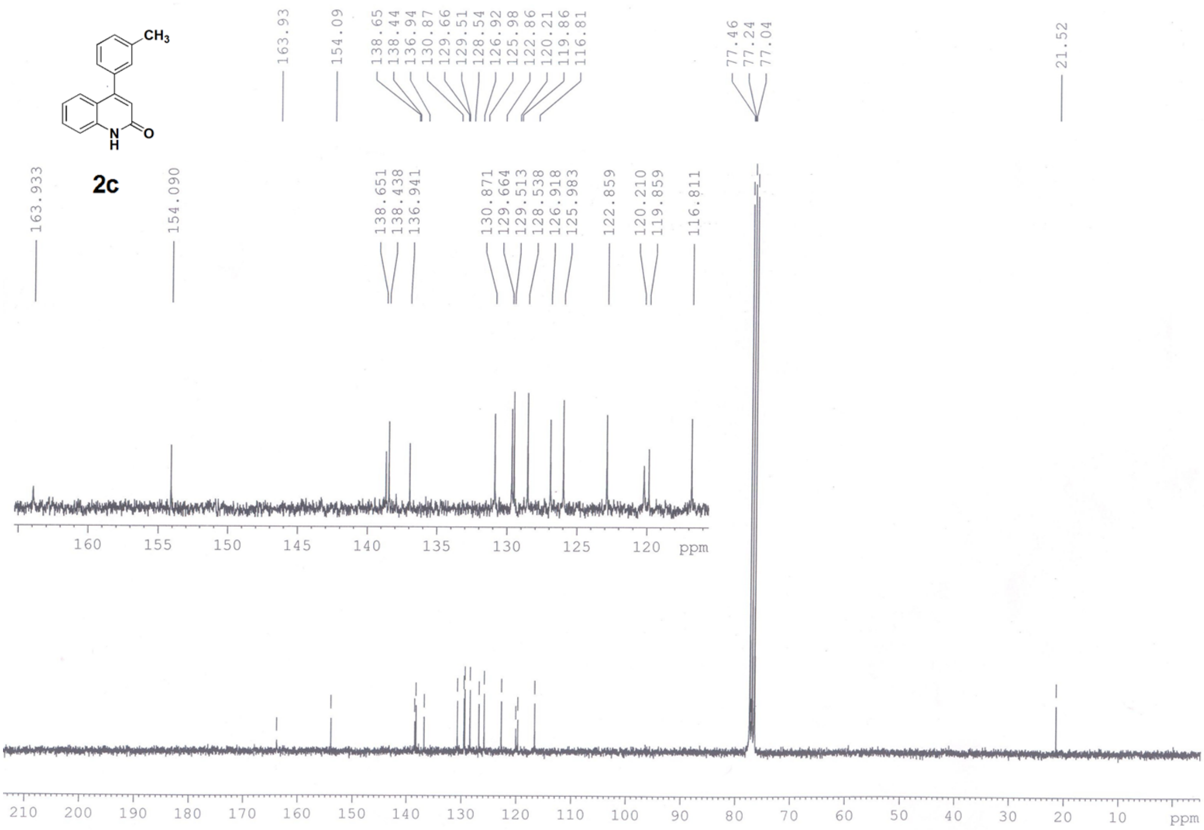
^{1}H and ^{13}C NMR spectra of 2b



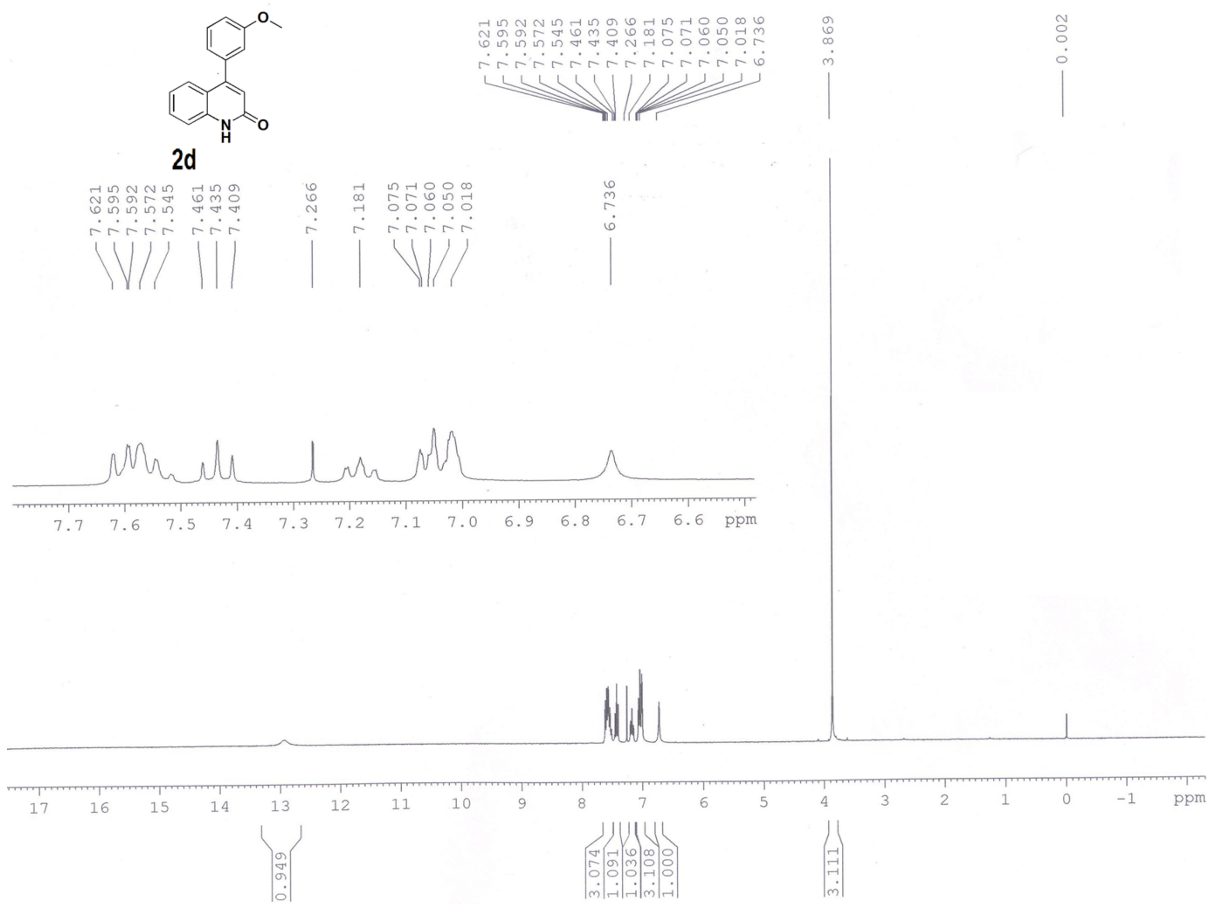


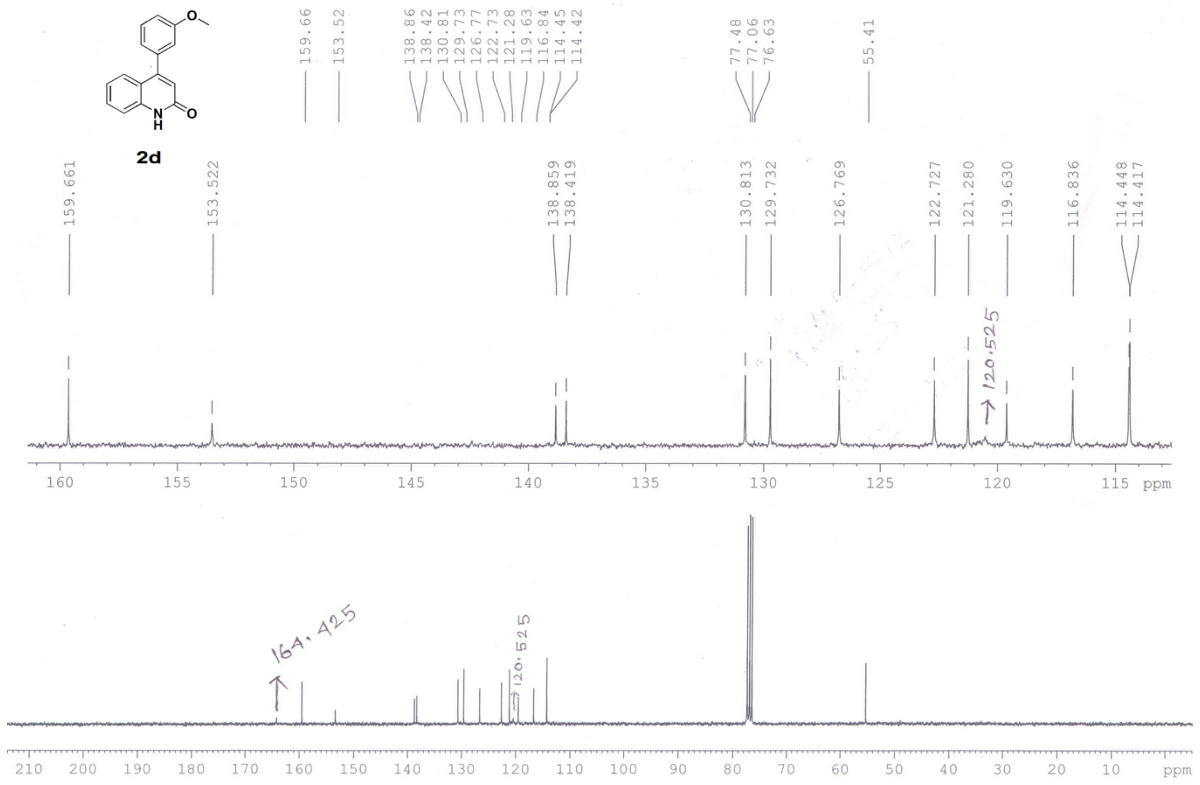
[1]H and [13]C NMR spectra of 2c



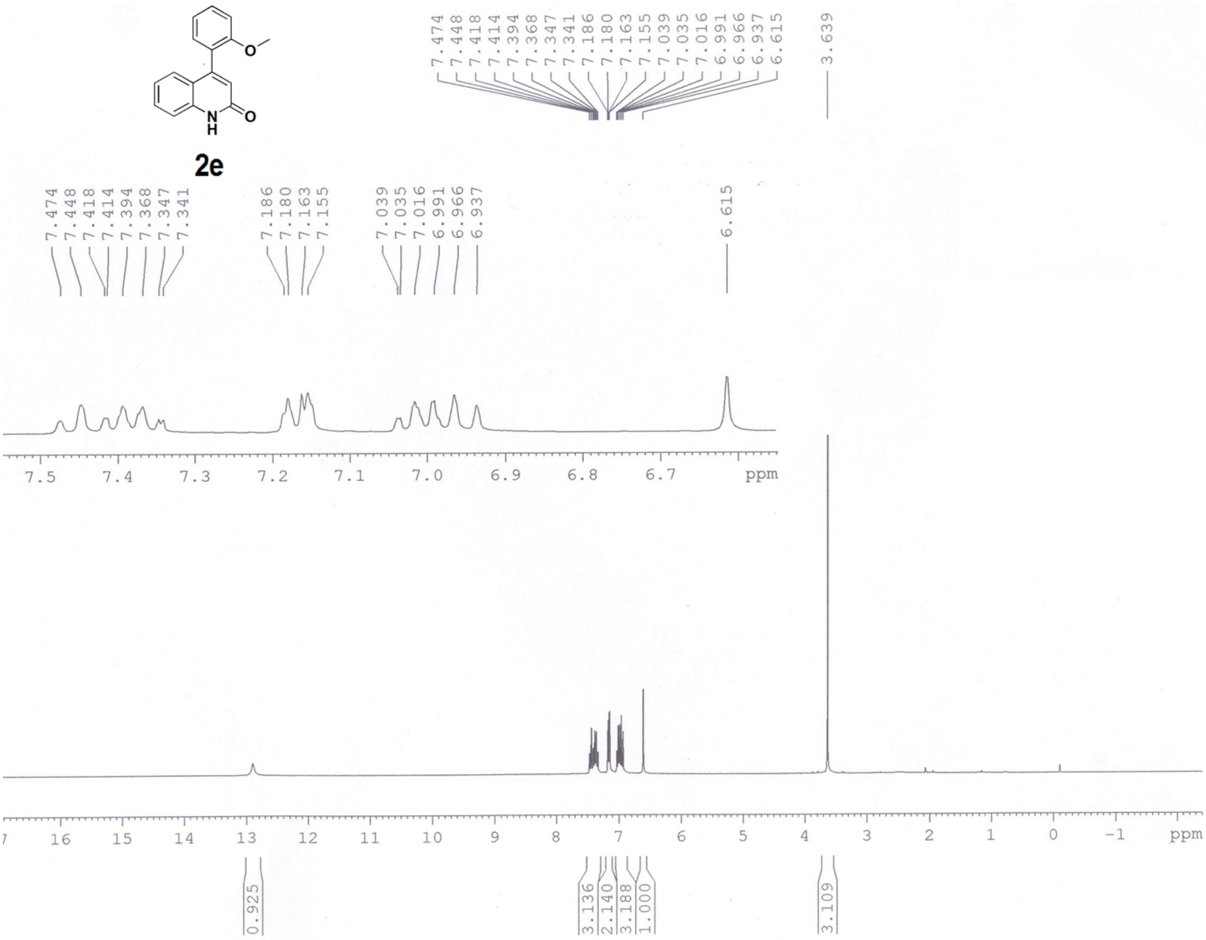


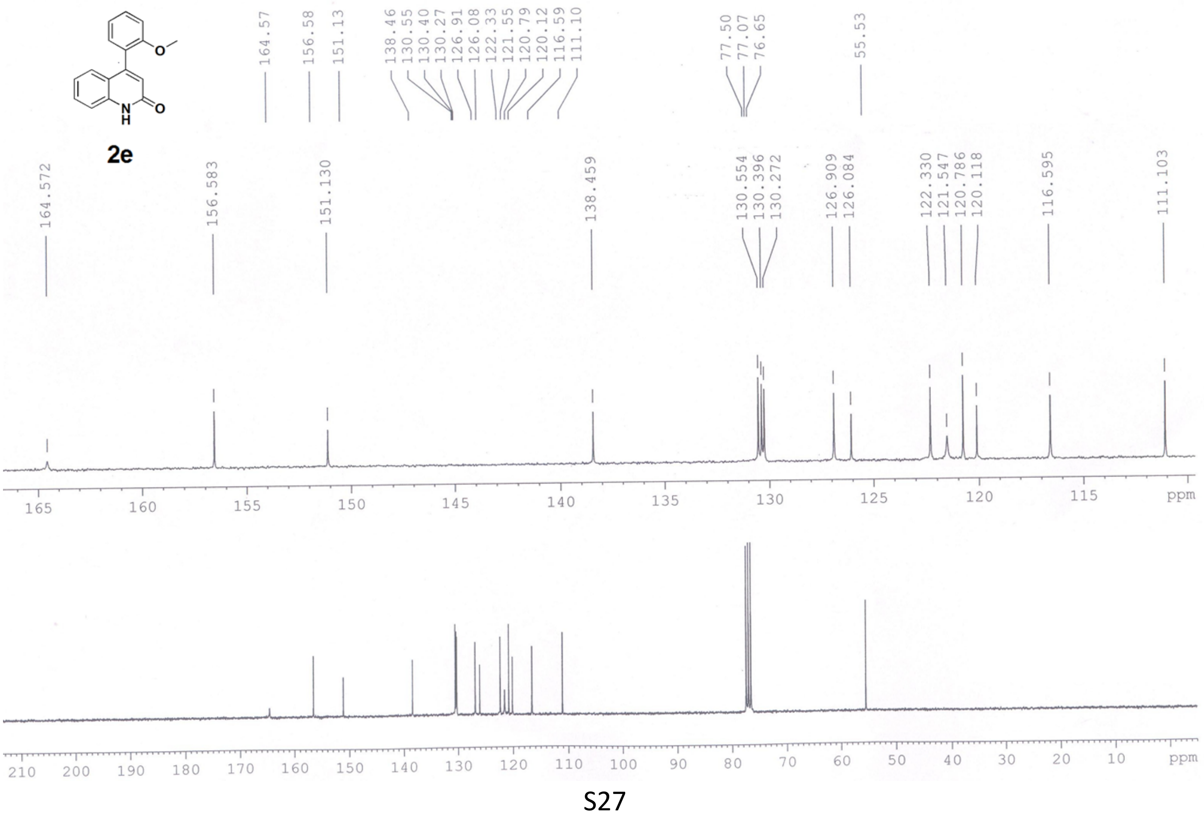
^{1}H and ^{13}C NMR spectra of 2d



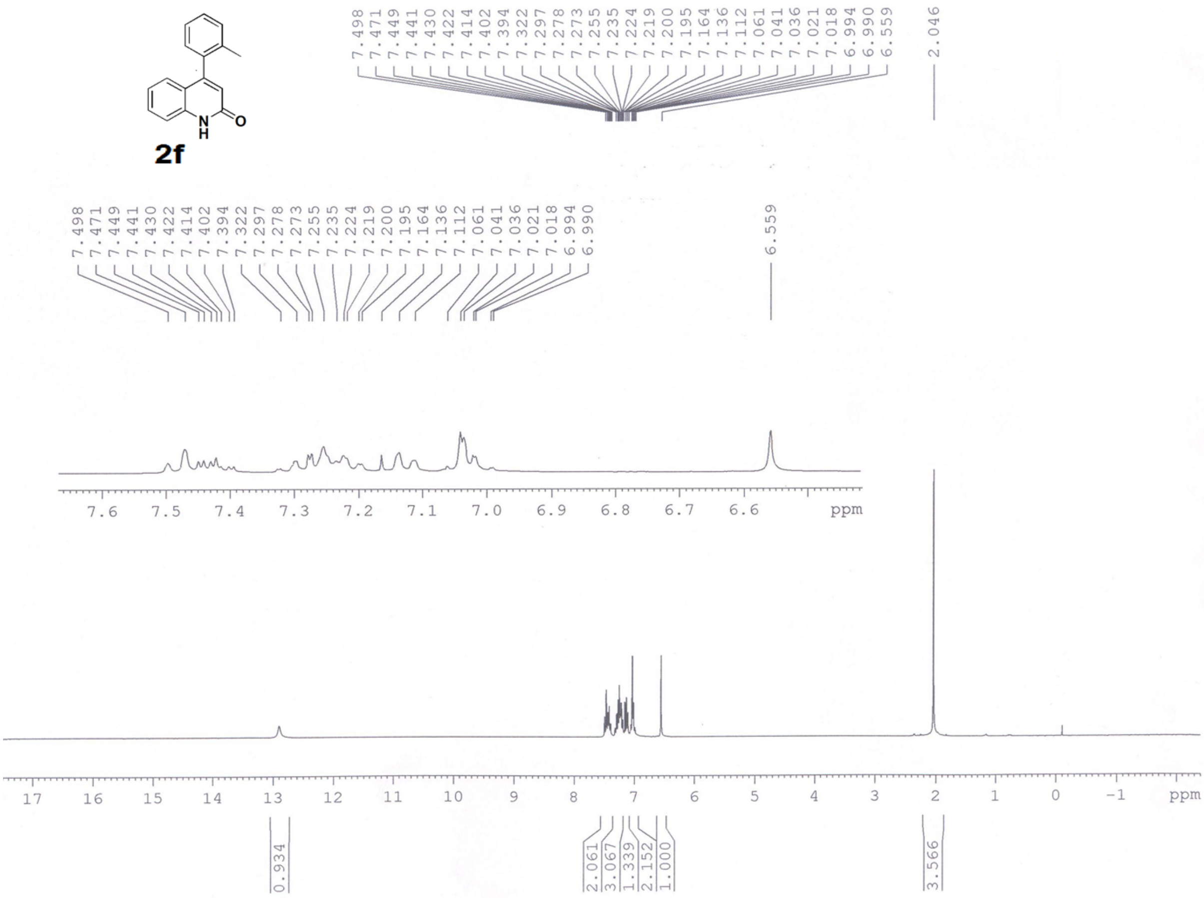


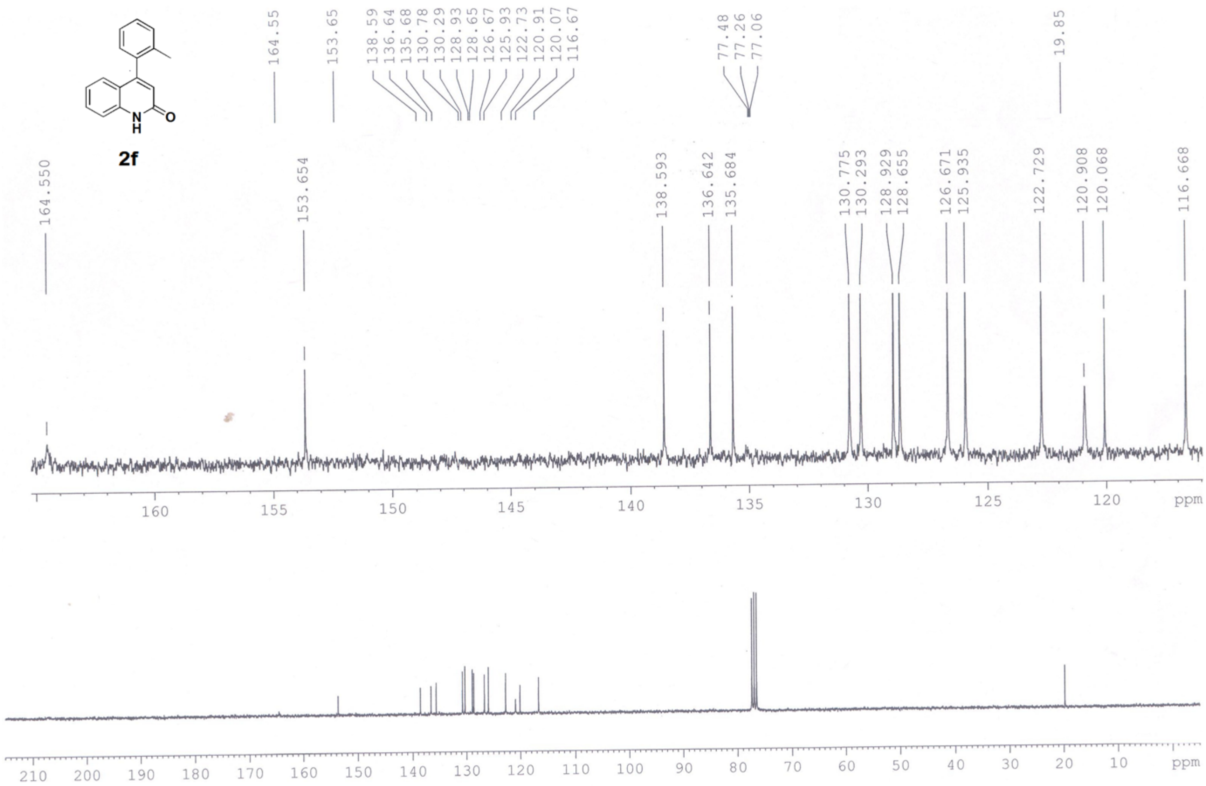
[1]H and [13]C NMR spectra of 2e





[1]H and [13]C NMR spectra of 2f





[1]H and [13]C NMR spectra of 2g